J Andrs

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Graphene Nanoplatelets: In Vivo and In Vitro Toxicity, Cell Proliferative Activity, and Cell Gene Expression. *Applied Sciences (Switzerland)*, **2022**, 12, 720	2.6	3
480	Ag2WO4 under microwave, electron beam and femtosecond laser irradiations: Unveiling the relationship between morphology and photoluminescence emissions. *Journal of Alloys and Compounds*, **2022**, 903, 163840	5.7	1
479	Interface matters: Design of an efficient Ag2WO4/Ag3PO4 photocatalyst. *Materials Chemistry and Physics*, **2022**, 280, 125710	4.4	0
478	Tailoring Bi2MoO6 by Eu3+ incorporation for enhanced photoluminescence emissions. *Journal of Luminescence*, **2022**, 243, 118675	3.8	2
477	A diagnosis approach for semiconductor properties evaluation from ab initio calculations: Ag-based materials investigation. *Journal of Solid State Chemistry*, **2022**, 305, 122670	3.3	0
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	5.1	0
475	Efficient Ni and Fe doping process in ZnO with enhanced photocatalytic activity: A theoretical and experimental investigation. *Materials Research Bulletin*, **2022**, 111849	5.1	6
474	Inactivation of SARS-CoV-2 by a chitosan/AgWO composite generated by femtosecond laser irradiation.. *Scientific Reports*, **2022**, 12, 8118	4.9	0
473	Formation of Metallic Ag on AgBr by Femtosecond Laser Irradiation. *Physchem*, **2022**, 2, 179-190		0
472	Protective Face Masks: Current Status and Future Trends. *ACS Applied Materials & Interfaces*, **2021**, 13, 56725-56751	9.5	16
471	Behavior of Bi2S3 under ultrasound irradiation for Rhodamine B dye degradation. *Chemical Physics Letters*, **2021**, 785, 139123	2.5	0
470	Selective Synthesis of and AgWO Polymorphs: Promising Platforms for Photocatalytic and Antibacterial Materials. *Inorganic Chemistry*, **2021**, 60, 1062-1079	5.1	8
469	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	13.1	6
468	Structure, Photoluminescence Emissions, and Photocatalytic Activity of AgSeO: A Joint Experimental and Theoretical Investigation. *Inorganic Chemistry*, **2021**, 60, 5937-5954	5.1	1
467	SiO-Ag Composite as a Highly Virucidal Material: A Roadmap that Rapidly Eliminates SARS-CoV-2. *Nanomaterials*, **2021**, 11,	5.4	19
466	A scalable electron beam irradiation platform applied for allotropic carbon transformation. *Carbon*, **2021**, 174, 567-580	10.4	3
465	Surface-dependent photocatalytic and biological activities of Ag2CrO4: Integration of experiment and simulation. *Applied Surface Science*, **2021**, 545, 148964	6.7	8

464	Identifying and explaining vibrational modes of sanbornite (low-BaSiO) and BaSiO: A joint experimental and theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 248, 119130	4.4	3
463	Modulating the properties of multifunctional semiconductors by means of morphology: Theory meets experiments. *Computational Materials Science*, **2021**, 188, 110217	3.2	8
462	Revealing the Nature of Defects in Ag2WO4 by Positron Annihilation Lifetime Spectroscopy: A Joint Experimental and Theoretical Study. *Crystal Growth and Design*, **2021**, 21, 1093-1102	3.5	4
461	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	8.3	6
460	PVC-SiO2-Ag composite as a powerful biocide and anti-SARS-CoV-2 material. *Journal of Polymer Research*, **2021**, 28, 1	2.7	4
459	Increasing the photocatalytic and fungicide activities of Ag3PO4 microcrystals under visible-light irradiation. *Ceramics International*, **2021**, 47, 22604-22614	5.1	1
458	Unveiling the Ag-Bi miscibility at the atomic level: A theoretical insight. *Computational Materials Science*, **2021**, 197, 110612	3.2	1
457	Carbon Nanofibers versus Silver Nanoparticles: Time-Dependent Cytotoxicity, Proliferation, and Gene Expression. *Biomedicines*, **2021**, 9,	4.8	4
456	Bioactive AgPO/Polypropylene Composites for Inactivation of SARS-CoV-2 and Other Important Public Health Pathogens. *Journal of Physical Chemistry B*, **2021**, 125, 10866-10875	3.4	0
455	Microwave-Driven Hexagonal-to-Monoclinic Transition in BiPO: An In-Depth Experimental Investigation and First-Principles Study. *Inorganic Chemistry*, **2020**, 59, 7453-7468	5.1	12
454	Surface-dependent properties of Ag2WO4: a joint experimental and theoretical investigation. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	10
453	Zinc-substituted Ag2CrO4: A material with enhanced photocatalytic and biological activity. *Journal of Alloys and Compounds*, **2020**, 835, 155315	5.7	9
452	Electron beam irradiation for the formation of thick Ag film on AgPO.. *RSC Advances*, **2020**, 10, 21745-21753	3.7	6
451	Metallic behavior in STO/LAO heterostructures with non-uniformly atomic interfaces. *Materials Today Communications*, **2020**, 24, 101339	2.5	0
450	Femtosecond-laser-irradiation-induced structural organization and crystallinity of BiWO. *Scientific Reports*, **2020**, 10, 4613	4.9	3
449	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	4.6	3
448	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	6.7	11
447	Unvealing the role of AgMoO microcrystals to the improvement of antibacterial activity. *Materials Science and Engineering C*, **2020**, 111, 110765	8.3	23

446	Connecting the surface structure, morphology and photocatalytic activity of Ag2O: An in depth and unified theoretical investigation. *Applied Surface Science*, **2020**, 509, 145321	6.7	29
445	Ag Nanoparticles/AgX (X=Cl, Br and I) Composites with Enhanced Photocatalytic Activity and Low Toxicological Effects. *ChemistrySelect*, **2020**, 5, 4655-4673	1.8	9
444	Towards a white-emitting phosphor Ca10V6O25 based material. *Journal of Luminescence*, **2020**, 220, 116990	3.8	2
443	Structure, electronic properties, morphology evolution, and photocatalytic activity in PbMoO and PbCaSrMoO (= 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions. *Physical Chemistry Chemical Physics*, **2020**, 22, 25876-25891	3.6	8
442	Toward Expanding the Optical Response of Ag2CrO4 and Bi2O3 by Their Laser-Mediated Heterojunction. *Journal of Physical Chemistry C*, **2020**, 124, 26404-26414	3.8	2
441	Structure, optical properties, and photocatalytic activity of Ag2W0.75Mo0.25O4. *Materials Research Bulletin*, **2020**, 132, 111011	5.1	4
440	Deciphering the Curly Arrow Representation and Electron Flow for the 1,3-Dipolar Rearrangement between Acetonitrile Oxide and (1,2,4)-2-Cyano-7-oxabicyclo[2.2.1]hept-5-en-2-yl Acetate Derivatives. *ACS Omega*, **2020**, 5, 22215-22225	3.9	3
439	Rational Design of W-Doped AgPO as an Efficient Antibacterial Agent and Photocatalyst for Organic Pollutant Degradation. *ACS Omega*, **2020**, 5, 23808-23821	3.9	6
438	Unraveling the relationship between exposed surfaces and the photocatalytic activity of AgPO: an in-depth theoretical investigation.. *RSC Advances*, **2020**, 10, 30640-30649	3.7	6
437	Unconventional Magnetization Generated from Electron Beam and Femtosecond Irradiation on AgWO: A Quantum Chemical Investigation. *ACS Omega*, **2020**, 5, 10052-10067	3.9	8
436	Unveiling the efficiency of microwave-assisted hydrothermal treatment for the preparation of SrTiO mesocrystals. *Physical Chemistry Chemical Physics*, **2019**, 21, 22031-22038	3.6	6
435	In Situ Growth of Bi Nanoparticles on NaBiO3, and Bi2O3 Surfaces: Electron Irradiation and Theoretical Insights. *Journal of Physical Chemistry C*, **2019**, 123, 5023-5030	3.8	10
434	How effectively bonding evolution theory retrieves and visualizes curly arrows: The cycloaddition reaction of cyclic nitrones. *International Journal of Quantum Chemistry*, **2019**, 119, e25985	2.1	9
433	AgVO Decorated by Hydroxyapatite (Ca(PO)(OH)): Tuning Its Photoluminescence Emissions and Bactericidal Activity. *Inorganic Chemistry*, **2019**, 58, 5900-5913	5.1	9
432	Proof-of-Concept Studies Directed toward the Formation of Metallic Ag Nanostructures from Ag3PO4 Induced by Electron Beam and Femtosecond Laser. *Particle and Particle Systems Characterization*, **2019**, 36, 1800533	3.1	9
431	Connecting Theory with Experiment to Understand the Sintering Processes of Ag Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 11310-11318	3.8	8
430	Laser and electron beam-induced formation of Ag/Cr structures on AgCrO. *Physical Chemistry Chemical Physics*, **2019**, 21, 6101-6111	3.6	15
429	Geometry, electronic structure, morphology, and photoluminescence emissions of BaW1-xMoxO4 (x = 0, 0.25, 0.50, 0.75, and 1) solid solutions: Theory and experiment in concert. *Applied Surface Science*, **2019**, 463, 907-917	6.7	15

428	Computational procedure to an accurate DFT simulation to solid state systems. *Computational Materials Science*, **2019**, 170, 109176	3.2	7
427	Joint Theoretical and Experimental Study on the La Doping Process in InO: Phase Transition and Electrocatalytic Activity. *Inorganic Chemistry*, **2019**, 58, 11738-11750	5.1	15
426	On the catalytic transfer hydrogenation of nitroarenes by a cubane-type MoS cluster hydride: disentangling the nature of the reaction mechanism. *Physical Chemistry Chemical Physics*, **2019**, 21, 17221-17231	3.6	4
425	Ag Nanoparticles/AgWO Composite Formed by Electron Beam and Femtosecond Irradiation as Potent Antifungal and Antitumor Agents. *Scientific Reports*, **2019**, 9, 9927	4.9	24
424	Evidence for the formation of metallic In after laser irradiation of InP. *Journal of Applied Physics*, **2019**, 126, 025902	2.5	2
423	Understanding the White-Emitting CaMoO4 Co-Doped Eu3+, Tb3+, and Tm3+ Phosphor through Experiment and Computation. *Journal of Physical Chemistry C*, **2019**, 123, 18536-18550	3.8	27
422	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
421	Designing biocompatible and multicolor fluorescent hydroxyapatite nanoparticles for cell-imaging applications. *Materials Today Chemistry*, **2019**, 14, 100211	6.2	7
420	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	5.5	11
419	First principle investigation of the exposed surfaces and morphology of ZnMoO4. *Journal of Applied Physics*, **2019**, 126, 235301	2.5	10
418	Polymorphs of ZnV2O6 under Pressure: A First-Principle Investigation. *Journal of Physical Chemistry C*, **2019**, 123, 3239-3253	3.8	11
417	Tailoring the Bactericidal Activity of Ag Nanoparticles/AgWO Composite Induced by Electron Beam and Femtosecond Laser Irradiation: Integration of Experiment and Computational Modeling.. *ACS Applied Bio Materials*, **2019**, 2, 824-837	4.1	25
416	Towards enhancing the magnetic properties by morphology control of ATiO3 (A = Mn, Fe, Ni) multiferroic materials. *Journal of Magnetism and Magnetic Materials*, **2019**, 475, 544-549	2.8	24
415	Structure, morphology and photoluminescence emissions of ZnMoO4: RE 3+=Tb3+ - Tm3+ - X Eu3+ (x= 1, 1.5, 2, 2.5 and 3 mol%) particles obtained by the sonochemical method. *Journal of Alloys and Compounds*, **2018**, 750, 55-70	5.7	26
414	Laser-induced formation of bismuth nanoparticles. *Physical Chemistry Chemical Physics*, **2018**, 20, 13693-13696	3.6	15
413	Towards the scale-up of the formation of nanoparticles on AgWO with bactericidal properties by femtosecond laser irradiation. *Scientific Reports*, **2018**, 8, 1884	4.9	32
412	Can Supported Reduced Vanadium Oxides form H from CHOH? A Computational Gas-Phase Mechanistic Study. *Journal of Physical Chemistry A*, **2018**, 122, 1104-1113	2.8	5
411	ZnWO nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 1923-1937	3.6	77

410	and AgVO3 polymorphs as photoluminescent materials: An example of temperature-driven synthesis. *Ceramics International*, **2018**, 44, 5939-5944	5.1	13
409	Binding free energy calculations to rationalize the interactions of huprines with acetylcholinesterase. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 607-622	4.2	2
408	Improving the ozone gas-sensing properties of CuWO4 nanoparticles. *Journal of Alloys and Compounds*, **2018**, 748, 411-417	5.7	33
407	Surfactant-Mediated Morphology and Photocatalytic Activity of Ag2WO4 Material. *Journal of Physical Chemistry C*, **2018**, 122, 8667-8679	3.8	45
406	Structural properties and self-activated photoluminescence emissions in hydroxyapatite with distinct particle shapes. *Ceramics International*, **2018**, 44, 236-245	5.1	21
405	Cuboidal Mo3S4 Clusters as a Platform for Exploring Catalysis: A Three-Center Sulfur Mechanism for Alkyne Semihydrogenation. *ACS Catalysis*, **2018**, 8, 7346-7350	13.1	9
404	Connecting structural, optical, and electronic properties and photocatalytic activity of Ag3PO4:Mo complemented by DFT calculations. *Applied Catalysis B: Environmental*, **2018**, 238, 198-211	21.8	39
403	Magnetism and multiferroic properties at MnTiO3 surfaces: A DFT study. *Applied Surface Science*, **2018**, 452, 463-472	6.7	32
402	Chemical Bond Formation and Rupture Processes: An Application of DFT Chemical Pressure Approach. *Journal of Physical Chemistry C*, **2018**, 122, 21216-21225	3.8	4
401	From Complex Inorganic Oxides to Ag-Bi Nanoalloy: Synthesis by Femtosecond Laser Irradiation. *ACS Omega*, **2018**, 3, 9880-9887	3.9	13
400	Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO3:Eu3+. *CrystEngComm*, **2018**, 20, 5519-5530	3.3	17
399	Experimental and theoretical study to explain the morphology of CaMoO 4 crystals. *Journal of Physics and Chemistry of Solids*, **2018**, 114, 141-152	3.9	31
398	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from first-principles calculations. *International Journal of Quantum Chemistry*, **2018**, 118, e25551	2.1	18
397	Theoretical approach for determining the relation between the morphology and surface magnetism of Co3O4. *Journal of Magnetism and Magnetic Materials*, **2018**, 453, 262-267	2.8	30
396	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of CaVO. *Inorganic Chemistry*, **2018**, 57, 15489-15499	5.1	15
395	Direct preparation of standard functional interfaces in oxide heterostructures for 2DEG analysis through beam-induced platinum contacts. *Applied Physics Letters*, **2018**, 113, 131603	3.4	1
394	In situ Formation of Metal Nanoparticles through Electron Beam Irradiation: Modeling Real Materials from First-Principles Calculations. *Journal of Material Science & Engineering*, **2018**, 07,	0.7	3
393	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	3.1	11

392	A DFT investigation of the role of oxygen vacancies on the structural, electronic and magnetic properties of ATiO (A = Mn, Fe, Ni) multiferroic materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 28382-28392	3.6	17
391	Computational Modeling for the Ag Nanoparticle Coalescence Process: A Case of Surface Plasmon Resonance. *Journal of Physical Chemistry C*, **2017**, 121, 7030-7036	3.8	13
390	Synthesis and evaluation of Ag2WO4 as novel antifungal agent. *Chemical Physics Letters*, **2017**, 674, 125-129	2.5	22
389	Synthesis of Cuboctahedral CeO2 Nanoclusters and Their Assembly into Cuboid Nanoparticles by Oriented Attachment. *ChemNanoMat*, **2017**, 3, 228-232	3.5	4
388	The interplay between morphology and photocatalytic activity in ZnO and N-doped ZnO crystals. *Materials and Design*, **2017**, 120, 363-375	8.1	52
387	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	6.1	24
386	Electronic structure and rearrangements of anionic [ClMg(2-O2C)] and [ClMg(2-CO2)] complexes: a quantum chemical topology study. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	5
385	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	3.6	19
384	AgZnWO (0 x 0.25) Solid Solutions: Structure, Morphology, and Optical Properties. *Inorganic Chemistry*, **2017**, 56, 7360-7372	5.1	26
383	Mechanism of Antibacterial Activity via Morphology Change of AgVO: Theoretical and Experimental Insights. *ACS Applied Materials & Interfaces*, **2017**, 9, 11472-11481	9.5	46
382	An experimental and theoretical investigation on the optical and photocatalytic properties of ZnS nanoparticles. *Journal of Physics and Chemistry of Solids*, **2017**, 103, 179-189	3.9	33
381	A novel approach to obtain highly intense self-activated photoluminescence emissions in hydroxyapatite nanoparticles. *Journal of Solid State Chemistry*, **2017**, 249, 64-69	3.3	16
380	Curly arrows, electron flow, and reaction mechanisms from the perspective of the bonding evolution theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 29031-29046	3.6	25
379	Tuning the Morphological, Optical, and Antimicrobial Properties of Ag2WO4 Microcrystals Using Different Solvents. *Crystal Growth and Design*, **2017**, 17, 6239-6246	3.5	27
378	First-Principles Study on Polymorphs of AgVO3: Assessing to Structural Stabilities and Pressure-Induced Transitions. *Journal of Physical Chemistry C*, **2017**, 121, 27624-27642	3.8	19
377	Bridging Structure and Real-Space Topology: Understanding Complex Molecules and Solid-State Materials **2017**, 427-454		2
376	Mechanism of photoluminescence in intrinsically disordered CaZrO3 crystals: First principles modeling of the excited electronic states. *Journal of Alloys and Compounds*, **2017**, 722, 981-995	5.7	15
375	Uncovering the metastable Ag2WO4 phase: a joint experimental and theoretical study. *RSC Advances*, **2017**, 7, 5610-5620	3.7	18

374	Photoluminescent properties of ZrO2: Tm3+, Tb3+, Eu3+ powders A combined experimental and theoretical study. *Journal of Alloys and Compounds*, **2017**, 695, 3094-3103	5.7	36
373	A bonding evolution analysis for the thermal Claisen rearrangement: an experimental and theoretical exercise for testing the electron density flow. *Physical Chemistry Chemical Physics*, **2017**, 20, 535-541	3.6	9
372	Formation of Ag Nanoparticles on Ag2WO4 through Electron Beam Irradiation: A Synergetic Computational and Experimental Study. *Inorganic Chemistry*, **2016**, 55, 8661-71	5.1	33
371	In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. *Scientific Reports*, **2016**, 6, 21498	4.9	32
370	Photoluminescence and Photocatalytic Properties of Ag PO Microcrystals: An Experimental and Theoretical Investigation. *ChemPlusChem*, **2016**, 81, 202-212	2.8	52
369	Synthesis, antifungal evaluation and optical properties of silver molybdate microcrystals in different solvents: a combined experimental and theoretical study. *Dalton Transactions*, **2016**, 45, 10736-43	4.3	38
368	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	1.9	3
367	Formation of Ag nanoparticles on metastable Ag2WO4 microcrystals induced by electron irradiation. *Chemical Physics Letters*, **2016**, 644, 68-72	2.5	27
366	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
365	Synthesis and characterization of metastable Ag2WO4: an experimental and theoretical approach. *Dalton Transactions*, **2016**, 45, 1185-91	4.3	18
364	Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 257-294	0.7	2
363	Disclosing the electronic structure and optical properties of Ag4V2O7 crystals: experimental and theoretical insights. *CrystEngComm*, **2016**, 18, 6483-6491	3.3	13
362	Effects of chemical substitution on the structural and optical properties of Ag2-2xNixWO4 (0 x 0.08) solid solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 21966-75	3.6	16
361	An Experimental and Computational Study of AgVO3: Optical Properties and Formation of Ag Nanoparticles. *Journal of Physical Chemistry C*, **2016**, 120, 12254-12264	3.8	37
360	In situ growth of Ag nanoparticles on Ag2WO4 under electron irradiation: probing the physical principles. *Nanotechnology*, **2016**, 27, 225703	3.4	28
359	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
358	Understanding the formation and growth of Ag nanoparticles on silver chromate induced by electron irradiation in electron microscope: A combined experimental and theoretical study. *Journal of Solid State Chemistry*, **2016**, 239, 220-227	3.3	21
357	Synthesis and morphological transformation of BaWO4 crystals: Experimental and theoretical insights. *Ceramics International*, **2016**, 42, 10913-10921	5.1	40

356	Acetone gas sensor based on Ag2WO4 nanorods obtained via a microwave-assisted hydrothermal route. *Journal of Alloys and Compounds*, **2016**, 683, 186-190	5.7	54
355	On the morphology of BaMoO4 crystals: A theoretical and experimental approach. *Crystal Research and Technology*, **2016**, 51, 634-644	1.3	16
354	Modeling the atomic-scale structure, stability, and morphological transformations in the tetragonal phase of LaVO4. *Chemical Physics Letters*, **2016**, 660, 87-92	2.5	28
353	Theoretical and Experimental Insight on Ag2CrO4 Microcrystals: Synthesis, Characterization, and Photoluminescence Properties. *Inorganic Chemistry*, **2016**, 55, 8961-70	5.1	27
352	A joint experimental and theoretical study on the electronic structure and photoluminescence properties of Al2(WO4)3 powders. *Journal of Molecular Structure*, **2015**, 1081, 381-388	3.4	18
351	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, 1470-80	6.4	12
350	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
349	Fingerprints of short-range and long-range structure in BaZr(1-x)HfxO3 solid solutions: an experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2015**, 17, 11341-9	3.6	9
348	Quantum chemical topological analysis of hydrogen bonding in HX⋯X and CH3X⋯X dimers (X = Br, Cl, F). *Molecular Simulation*, **2015**, 41, 600-609	2	7
347	Chemical structure and reactivity by means of quantum chemical topology analysis. *Computational and Theoretical Chemistry*, **2015**, 1053, 17-30	2	53
346	Chemical Bonding under Pressure **2015**, 131-157		
345	A Combined Experimental and Theoretical Study on the Formation of Ag Filaments on Ag2MoO4 Induced by Electron Irradiation. *Particle and Particle Systems Characterization*, **2015**, 32, 646-651	3.1	41
344	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
343	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
342	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
341	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*	7.1	52
340	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, 32358-74	3.6	7
339	Structural and optical properties of ZnS/MgNb2O6 heterostructures. *Superlattices and Microstructures*, **2015**, 79, 180-192	2.8	6

338	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
337	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
336	Unraveling reaction mechanisms by means of Quantum Chemical Topology Analysis. *International Journal of Quantum Chemistry*, **2014**, 114, 1239-1252	2.1	60
335	A novel ozone gas sensor based on one-dimensional (1D) AgWO nanostructures. *Nanoscale*, **2014**, 6, 4058-62	7.7	92
334	Potentiated electron transference in Ag2WO4 microcrystals with Ag nanofilaments as microbial agent. *Journal of Physical Chemistry A*, **2014**, 118, 5769-78	2.8	91
333	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	2.7	16
332	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
331	Correlation between structural and electronic order disorder effects and optical properties in ZnO nanocrystals. *Journal of Materials Chemistry C*, **2014**, 2, 10164-10174	7.1	26
330	Prediction of dopant atom distribution on nanocrystals using thermodynamic arguments. *Physical Chemistry Chemical Physics*, **2014**, 16, 1089-94	3.6	8
329	Oxygen atom transfer reactions from Mimoun complexes to sulfides and sulfoxides. A bonding evolution theory analysis. *Journal of Physical Chemistry A*, **2014**, 118, 6092-103	2.8	11
328	First-Principles Study of Pressure-Induced Phase Transitions and Electronic Properties of Ag2MoO4. *Journal of Physical Chemistry C*, **2014**, 118, 3724-3732	3.8	42
327	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
326	A DFT Study of Structural and Electronic Properties of ZnS Polymorphs and its Pressure-Induced Phase Transitions. *Journal of the American Ceramic Society*, **2014**, 97, 4011-4018	3.8	31
325	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
324	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
323	Flexural behavior and water absorption of asymmetrical sandwich composites from natural fibers and cork agglomerate core. *Materials Letters*, **2014**, 127, 48-52	3.3	32
322	Effect of polyvinyl alcohol on the shape, photoluminescence and photocatalytic properties of PbMoO4 microcrystals. *Materials Science in Semiconductor Processing*, **2014**, 26, 425-430	4.3	20
321	Silver Molybdate and Silver Tungstate Nanocomposites with Enhanced Photoluminescence. *Nanomaterials and Nanotechnology*, **2014**, 4, 22	2.9	72

320	Quantum mechanical modeling of excited electronic states and their relationship to cathodoluminescence of BaZrO3. *Journal of Applied Physics*, **2013**, 114, 043714	2.5	15
319	Microwave-hydrothermal synthesis of single-crystalline Co3O4 spinel nanocubes. *CrystEngComm*, **2013**, 15, 7443	3.3	33
318	A combined theoretical and experimental study of electronic structure and optical properties of ZnMoO4 microcrystals. *Polyhedron*, **2013**, 54, 13-25	2.7	65
317	Direct in situ observation of the electron-driven synthesis of Ag filaments on Ag2WO4 crystals. *Scientific Reports*, **2013**, 3, 1676	4.9	95
316	Synthesis of wurtzite ZnS nanoparticles using the microwave assisted solvothermal method. *Journal of Alloys and Compounds*, **2013**, 556, 153-159	5.7	78
315	Structural refinement, growth mechanism, infrared/Raman spectroscopies and photoluminescence properties of PbMoO4 crystals. *Polyhedron*, **2013**, 50, 532-545	2.7	57
314	Experimental and theoretical approach of nanocrystalline TiO2 with antifungal activity. *Chemical Physics Letters*, **2013**, 577, 114-120	2.5	13
313	New insight into the electronic structure of iron(IV)-oxo porphyrin compound I. A quantum chemical topological analysis. *Journal of Computational Chemistry*, **2013**, 34, 780-9	3.5	3
312	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
311	Toward an understanding of the hydrogenation reaction of MO2 gas-phase clusters (M = Ti, Zr, and Hf). *Journal of Physical Chemistry A*, **2013**, 117, 5354-64	2.8	10
310	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
309	Manufacture of Green-Composite Sandwich Structures with Basalt Fiber and Bioepoxy Resin. *Advances in Materials Science and Engineering*, **2013**, 2013, 1-9	1.5	19
308	Towards an Understanding on the Role of Precursor in the Synthesis of ZnS Nanostructures. *Current Physical Chemistry*, **2013**, 3, 378-385	0.5	3
307	Nature of the ring-closure process along the rearrangement of octa-1,3,5,7-tetraene to cycloocta-1,3,5-triene from the perspective of the electron localization function and catastrophe theory. *Journal of Computational Chemistry*, **2012**, 33, 748-56	3.5	39
306	SnO2 nanocrystals synthesized by microwave-assisted hydrothermal method: towards a relationship between structural and optical properties. *Journal of Nanoparticle Research*, **2012**, 14, 1	2.3	42
305	Structural and Electronic Effects of Incorporating Mn in TiO2 Films Grown by Sputtering: Anatase versus Rutile. *Journal of Physical Chemistry C*, **2012**, 116, 8753-8762	3.8	27
304	Structural and Electronic Properties of Lithiated SnO2. A Periodic DFT Study. *Journal of Physical Chemistry C*, **2012**, 116, 16127-16137	3.8	14
303	Quantum Mechanics Insight into the Microwave Nucleation of SrTiO3 Nanospheres. *Journal of Physical Chemistry C*, **2012**, 116, 24792-24808	3.8	52

302	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, 2500-5	6.4	26
301	Electronic fluxes during Diels-Alder reactions involving 1,2-benzoquinones: mechanistic insights from the analysis of electron localization function and catastrophe theory. *Journal of Computational Chemistry*, **2012**, 33, 2400-11	3.5	21
300	CaSO4 and its pressure-induced phase transitions. A density functional theory study. *Inorganic Chemistry*, **2012**, 51, 1751-9	5.1	36
299	Electronic structure and magnetic properties of FeWO4 nanocrystals synthesized by the microwave-hydrothermal method. *Materials Characterization*, **2012**, 73, 124-129	3.9	19
298	Novel SrTi1?FexO3 nanocubes synthesized by microwave-assisted hydrothermal method. *CrystEngComm*, **2012**, 14, 4068	3.3	20
297	Synthesis, optical and ferroelectric properties of PZT thin films: experimental and theoretical investigation. *Journal of Materials Chemistry*, **2012**, 22, 6587		18
296	Photoluminescence Properties of Nanocrystals. *Journal of Nanomaterials*, **2012**, 2012, 1-2	3.2	3
295	Relationship between Crystal Shape, Photoluminescence, and Local Structure inSrTiO3Synthesized by Microwave-Assisted Hydrothermal Method. *Journal of Nanomaterials*, **2012**, 2012, 1-6	3.2	18
294	Hybrid schemes based on quantum mechanics/molecular mechanics simulations goals to success, problems, and perspectives. *Advances in Protein Chemistry and Structural Biology*, **2011**, 85, 81-142	5.3	18
293	Hierarchical Assembly of CaMoO4 Nano-Octahedrons and Their Photoluminescence Properties. *Journal of Physical Chemistry C*, **2011**, 115, 5207-5219	3.8	113
292	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
291	A Theoretical Study on the Pressure-Induced Phase Transitions in the Inverse Spinel Structure Zn2SnO4. *Journal of Physical Chemistry C*, **2011**, 115, 7740-7746	3.8	28
290	Effect of coverage and defects on the adsorption of propanethiol on Au(111) surface: a theoretical study. *Langmuir*, **2011**, 27, 14514-21	4	29
289	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO4 Crystals. *Journal of Physical Chemistry C*, **2011**, 115, 20113-20119	3.8	66
288	Anomalous oriented attachment growth behavior on SnO2 nanocrystals. *Chemical Communications*, **2011**, 47, 3117-9	5.8	32
287	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	0.6	4
286	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
285	A Thermodynamic Approach to Predict Dopant Atoms Segregation on Nanocrystals. *Microscopy and Microanalysis*, **2011**, 17, 1458-1459	0.5	

284	Radioluminescence properties of decaoctahedral BaZrO3. *Scripta Materialia*, **2011**, 64, 118-121	5.6	31
283	An improved method for preparation of SrTiO3 nanoparticles. *Materials Chemistry and Physics*, **2011**, 125, 168-173	4.4	63
282	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	2.7	7
281	Insight into Copper-Based Catalysts: Microwave-Assisted Morphosynthesis, In Situ Reduction Studies, and Dehydrogenation of Ethanol. *ChemCatChem*, **2011**, 3, 839-843	5.2	18
280	N, P, and As ylides and aza- and arsa-Wittig reactions from topological analyses of electron density. *Journal of Physical Chemistry A*, **2011**, 115, 8316-26	2.8	12
279	Olefin epoxidation by molybdenum peroxo compound: molecular mechanism characterized by the electron localization function and catastrophe theory. *Journal of Physical Chemistry A*, **2011**, 115, 514-22	2.8	22
278	Photolumiscent properties of nanorods and nanoplates Y2O3:Eu3+. *Journal of Fluorescence*, **2011**, 21, 1431-8	2.4	17
277	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. *Theoretical Chemistry Accounts*, **2011**, 128, 601-607	1.9	7
276	Dopant segregation analysis on Sb:SnO2 nanocrystals. *Chemistry - A European Journal*, **2011**, 17, 11515-9	4.8	18
275	On the reversed crystal growth of BaZrO3 decaoctahedron: shape evolution and mechanism. *CrystEngComm*, **2011**, 13, 5818	3.3	39
274	Efficient microwave-assisted hydrothermal synthesis of CuO sea urchin-like architectures via a mesoscale self-assembly. *CrystEngComm*, **2010**, 12, 1696	3.3	92
273	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
272	An efficient microwave-assisted hydrothermal synthesis of BaZrO3 microcrystals: growth mechanism and photoluminescence emissions. *CrystEngComm*, **2010**, 12, 3612	3.3	64
271	Unraveling the Mechanisms of the Selective Oxidation of Methanol to Formaldehyde in Vanadia Supported on Titania Catalyst. *Journal of Physical Chemistry C*, **2010**, 114, 6039-6046	3.8	19
270	General and Theoretical Aspects of the Metal Enolates **2010**,		1
269	A theoretical study on the photoluminescence of SrTiO3. *Chemical Physics Letters*, **2010**, 493, 141-146	2.5	41
268	Theoretical QM/MM studies of enzymatic pericyclic reactions. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 115-31	3.5	7
267	Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. *Journal of Computational Chemistry*, **2010**, 31, 2493-501	3.5	11

266	Electronic structure and optical properties of BaMoO4 powders. *Current Applied Physics*, **2010**, 10, 614-624	2.6	130
265	First principles calculations on the origin of violet-blue and green light photoluminescence emission in SrZrO3 and SrTiO3 perovskites. *Theoretical Chemistry Accounts*, **2009**, 124, 385-394	1.9	63
264	Photoluminescent behavior of SrZrO3/SrTiO3 multilayer thin films. *Chemical Physics Letters*, **2009**, 473, 293-298	2.5	27
263	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	2.5	6
262	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
261	Mechanism and plasticity of isochorismate pyruvate lyase: a computational study. *Journal of the American Chemical Society*, **2009**, 131, 16156-61	16.4	26
260	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, 3032-8	6.4	28
259	Unveiling the chemical and morphological features of Sb-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, 14544-8	16.4	52
258	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
257	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, 7189-96	3.6	9
256	Morphology and Blue Photoluminescence Emission of PbMoO4 Processed in Conventional Hydrothermal. *Journal of Physical Chemistry C*, **2009**, 113, 5812-5822	3.8	156
255	A theoretical study on the mechanism of the base-promoted decomposition of N-chloro,N-methylethanolamine. *Organic and Biomolecular Chemistry*, **2009**, 7, 1807-14	3.9	5
254	A quantum mechanic/molecular mechanic study of the wild-type and N155S mutant HIV-1 integrase complexed with diketo acid. *Biophysical Journal*, **2008**, 94, 2443-51	2.9	22
253	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
252	Computational design of biological catalysts. *Chemical Society Reviews*, **2008**, 37, 2634-43	58.5	36
251	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
250	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
249	Strain behavior of lanthanum modified BiFeO3 thin films prepared via soft chemical method. *Journal of Applied Physics*, **2008**, 104, 104115	2.5	35

248	Intercalation processes and diffusion paths of lithium ions in spinel-type structured Li1+xTi2O4: Density functional theory study. *Physical Review B*, **2008**, 77,	3.3	22
247	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
246	Theoretical study on the reaction mechanism of VO2+ with propyne in gas phase. *Journal of Physical Chemistry A*, **2008**, 112, 1808-16	2.8	15
245	Synthesis and molecular and electronic structures of a series of Mo3CoSe4 cluster complexes with three different metal electron populations. *Inorganic Chemistry*, **2008**, 47, 3661-8	5.1	9
244	Origin of the absorption maxima of the photoactive yellow protein resolved via ab initio multiconfigurational methods. *Journal of Physical Chemistry B*, **2008**, 112, 7153-6	3.4	29
243	Predicting an improvement of secondary catalytic activity of promiscuous isochorismate pyruvate lyase by computational design. *Journal of the American Chemical Society*, **2008**, 130, 2894-5	16.4	22
242	An electron localization function and catastrophe theory analysis on the molecular mechanism of gas-phase identity SN2 reactions. *Theoretical Chemistry Accounts*, **2008**, 120, 341-349	1.9	33
241	Combined 13C NMR and DFT/GIAO studies of the polyketides Aurasperone A and Fonsecinone A. *International Journal of Quantum Chemistry*, **2008**, 108, 2408-2416	2.1	2
240	Theoretical study of catalytic efficiency of a Diels-Alderase catalytic antibody: an indirect effect produced during the maturation process. *Chemistry - A European Journal*, **2008**, 14, 596-602	4.8	8
239	Two state reactivity mechanism for the rearrangement of hydrogen peroxynitrite to nitric acid. *Chemical Physics Letters*, **2008**, 457, 216-221	2.5	12
238	Proton transport catalysis in intramolecular rearrangements: A density functional theory study. *Chemical Physics Letters*, **2008**, 464, 271-275	2.5	4
237	A DFT study of methanol dissociation on isolated vanadate groups. *Catalysis Today*, **2008**, 139, 214-220	5.3	16
236	A theoretical study on the electronic structure of Au-XO(0,-1,+1) (X=C, N, and O) complexes: effect of an external electric field. *Journal of Physical Chemistry A*, **2007**, 111, 13255-63	2.8	25
235	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, 816-23	6.4	29
234	Combined theoretical and experimental analysis of the bonding in the heterobimetallic cubane-type Mo(3)NiS(4) and Mo(3)CuS(4) core clusters. *Inorganic Chemistry*, **2007**, 46, 2159-66	5.1	19
233	Prediction of Gold Zigzag Nanotube-like Structure Based on Au32Units: A Quantum Chemical Study. *Journal of Physical Chemistry C*, **2007**, 111, 10342-10346	3.8	38
232	A quantum mechanics/molecular mechanics study of the protein-ligand interaction for inhibitors of HIV-1 integrase. *Chemistry - A European Journal*, **2007**, 13, 7715-24	4.8	36
231	Computer-aided rational design of catalytic antibodies: The 1F7 case. *Angewandte Chemie - International Edition*, **2007**, 46, 286-90	16.4	23

230	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. *Angewandte Chemie*, **2007**, 119, 290-294	3.6	2
229	New insights on the bridge carbon-carbon bond in propellanes: a theoretical study based on the analysis of the electron localization function. *Journal of Computational Chemistry*, **2007**, 28, 857-64	3.5	37
228	Nucleofugality index in □elimination reactions. *Chemical Physics Letters*, **2007**, 439, 177-182	2.5	24
227	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, 3818-24	3.4	17
226	Understanding the chemical reactivity of phenylhalocarbene systems: an analysis based on the spin-polarized density functional theory. *Theoretical Chemistry Accounts*, **2007**, 118, 325-335	1.9	15
225	Contribution of structural order-disorder to the green photoluminescence of PbWO4. *Physical Review B*, **2007**, 75,	3.3	44
224	Nucleophilicity index from perturbed electrostatic potentials. *Journal of Physical Chemistry A*, **2007**, 111, 2442-7	2.8	54
223	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
222	Oxygen adsorption on gold nanofacets and model clusters. *Journal of Chemical Physics*, **2006**, 125, 054703	3.9	41
221	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
220	Mechanistic Insights into the Reaction between VO2+ and Propene Based on a DFT Study. *Organometallics*, **2006**, 25, 1643-1653	3.8	28
219	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, 754-62	4.2	24
218	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
217	Stereoselectivity behavior of the AZ28 antibody catalyzed oxy-Cope rearrangement. *Journal of Physical Chemistry A*, **2006**, 110, 726-30	2.8	2
216	Catalysis in glycine N-methyltransferase: testing the electrostatic stabilization and compression hypothesis. *Biochemistry*, **2006**, 45, 14917-25	3.2	26
215	Molecular oxygen adsorption on electropositive nano gold tips. *Chemical Physics Letters*, **2006**, 421, 433-438	2.5	36
214	Homofugality: A new reactivity index describing the leaving group ability in homolytic substitution reactions. *Chemical Physics Letters*, **2006**, 424, 437-442	2.5	13
213	DFT study on the water-assisted mechanism for the reaction between VO+ and NH3 to yield VNH+ and H2O. *Chemical Physics Letters*, **2006**, 427, 265-270	2.5	5

212	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	2.5	4
211	A DFT study of the Diels□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	2.4	35
210	GENERALIZED DIABATIC STUDY OF ETHYLENE □SOMERISM□**2006**, 177-196		1
209	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
208	DFT study of oxygen adsorption on modified nanostructured gold pyramids. *Journal of Physical Chemistry B*, **2005**, 109, 7624-30	3.4	41
207	Room-temperature photoluminescence of BaTiO3: Joint experimental and theoretical study. *Physical Review B*, **2005**, 71,	3.3	93
206	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
205	Toward an understanding of the catalytic role of hydrogen-bond donor solvents in the hetero-Diels-Alder reaction between acetone and butadiene derivative. *Journal of Physical Chemistry A*, **2005**, 109, 10438-44	2.8	40
204	Exploring two-state reactivity pathways in the cycloaddition reactions of triplet methylene. *Journal of Physical Chemistry A*, **2005**, 109, 4178-84	2.8	9
203	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
202	Migration of the subsurface C impurity in Pd(111). *Physical Review B*, **2005**, 71,	3.3	38
201	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
200	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. *Tetrahedron*, **2005**, 61, 417-422	2.4	29
199	An electron localization function study of the trimerization of acetylene: Reaction mechanism and development of aromaticity. *Chemical Physics Letters*, **2005**, 406, 393-397	2.5	47
198	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	2.7	35
197	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, 1427-37	3.5	46
196	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	3.2	19
195	Lewis Acid Mediated Domino Reaction between 2-Cyclohexenone and Methyl Azide □A DFT Study. *European Journal of Organic Chemistry*, **2005**, 2005, 4705-4709	3.2	16

194	Towards a rational design of antibody catalysts through computational chemistry. *Angewandte Chemie - International Edition*, **2005**, 44, 904-9	16.4	9
193	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. *Angewandte Chemie*, **2005**, 117, 926-931	3.6	3
192	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	6	17
191	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	3.3	46
190	A theoretical analysis of the TiO2/Sn doped (1 1 0) surface properties. *Surface Science*, **2005**, 580, 71-79	1.8	41
189	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO[sub 3]. *Electrochemical and Solid-State Letters*, **2005**, 8, J21		9
188	DFT Study of the Reaction between VO2+ and C2H6. *Organometallics*, **2004**, 23, 730-739	3.8	61
187	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	2.1	31
186	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
185	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, 4742-9	4.8	26
184	Origin of photoluminescence in SrTiO3: a combined experimental and theoretical study. *Journal of Solid State Chemistry*, **2004**, 177, 3879-3885	3.3	57
183	DFT study of the water-assisted tautomerization process between hydrated oxide, MO(H2O)+, and dihydroxide, M(OH)2+, cations (M=V, Nb and Ta). *Chemical Physics Letters*, **2004**, 384, 56-62	2.5	24
182	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	2.8	7
181	Combined Experimental and Theoretical Study to Understand the Photoluminescence of Sr1-xTiO3-x. *Journal of Physical Chemistry B*, **2004**, 108, 9221-9227	3.4	36
180	A comparative study of claisen and cope rearrangements catalyzed by chorismate mutase. An insight into enzymatic efficiency: transition state stabilization or substrate preorganization?. *Journal of the American Chemical Society*, **2004**, 126, 311-9	16.4	40
179	A Theoretical Study on the Gas Phase Reactions of the Anions NbO3-, NbO5-, and NbO2(OH)2- with H2O and O2. *Journal of Physical Chemistry A*, **2004**, 108, 10850-10860	2.8	24
178	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
177	Theoretical insights in enzyme catalysis. *Chemical Society Reviews*, **2004**, 33, 98-107	58.5	129

176	Toward Understanding the Electron Density Distribution in Magnetic Clusters: Insight from the ELF and AIM Analyses of Ground-State Fe4. *Journal of Physical Chemistry A*, **2004**, 108, 6025-6031	2.8	22
175	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
174	Preorganization and reorganization as related factors in enzyme catalysis: the chorismate mutase case. *Chemistry - A European Journal*, **2003**, 9, 984-91	4.8	52
173	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		12
172	Electronic and structural properties of SnxTi1−xO2 solid solutions: a periodic DFT study. *Catalysis Today*, **2003**, 85, 145-152	5.3	66
171	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
170	Sulfide and sulfoxide oxidations by mono- and diperoxo complexes of molybdenum. A density functional study. *Journal of Organic Chemistry*, **2003**, 68, 5870-4	4.2	24
169	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
168	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
167	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
166	Crystal growth in colloidal tin oxide nanocrystals induced by coalescence at room temperature. *Applied Physics Letters*, **2003**, 83, 1566-1568	3.4	237
165	Understanding the mechanism of base-assisted decomposition of (N-halo),N-alkylalcoholamines. *Organic and Biomolecular Chemistry*, **2003**, 1, 4323-8	3.9	4
164	Thermodynamic argument about SnO2 nanoribbon growth. *Applied Physics Letters*, **2003**, 83, 635-637	3.4	105
163	A DFT Study of the Molecular Mechanisms of the Diels−Alder Reaction between Cyclopentadiene and 3-Phenyl-1-(2-pyridyl)-2-propen-1-one. Role of the Zn2+ Lewis Acid Catalyst and Water Solvent. *European Journal of Organic Chemistry*, **2002**, 2002, 2557	3.2	16
162	An atom-in-molecules and electron-localization-function study of the interaction between O2 and VxOy+/VxOy (x = 1, 2, y = 1−5) clusters. *Theoretical Chemistry Accounts*, **2002**, 108, 12-20	1.9	19
161	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		9
160	A joint theoretical and kinetic investigation on the fragmentation of (N-halo)-2-amino cycloalkanecarboxylates. *Chemical Physics*, **2002**, 280, 1-14	2.3	6
159	Author Index to Volumes 271−280. *Chemical Physics*, **2002**, 280, 1-26	2.3	3

158	Enzyme catalysis: Transition structures and quantum dynamical aspects: Modeling rubiscoIs oxygenation and carboxylation mechanisms. *International Journal of Quantum Chemistry*, **2002**, 88, 154-166	2.1	10
157	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	2.4	14
156	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
155	The nature of the AuRg bond in the [AuRg4]2+ (Rg=Ar, Kr and Xe) molecules. *Chemical Physics Letters*, **2002**, 356, 483-489	2.5	29
154	Quantum-mechanical simulation of MgAl2O4 under high pressure. *Physical Review B*, **2002**, 66,	3.3	37
153	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
152	Stability of MgAl 2 O 4 Under High-Pressure Conditions. *High Pressure Research*, **2002**, 22, 447-450	1.6	2
151	Topological analysis of the bonds in incomplete cuboidal [Mo3S4] clusters. *New Journal of Chemistry*, **2002**, 26, 844-850	3.6	35
150	Quantum Theory of Solvent Effects and Chemical Reactions **2002**, 283-361		1
149	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. *Theoretical Chemistry Accounts*, **2001**, 105, 207-212	1.9	40
148	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VOx and VOx+ (x=1 4) systems. *Theoretical Chemistry Accounts*, **2001**, 105, 299-308	1.9	63
147	Density functional study of the 5-methylcytosine tautomers. *Chemical Physics*, **2001**, 264, 333-340	2.3	32
146	Theoretical analysis on TiO2(110)/V surface. *International Journal of Quantum Chemistry*, **2001**, 85, 44-51	2.1	10
145	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
144	Electronic mechanistic pattern for C bond-breaking from transition structures in RubiscoIs chemistry. *Chemical Physics Letters*, **2001**, 340, 391-399	2.5	14
143	A B3LYP/6-31G** study on the chlorination of ammonia by hypochlorous acid. *Chemical Physics Letters*, **2001**, 342, 405-410	2.5	24
142	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. *Chemical Physics Letters*, **2001**, 338, 224-230	2.5	34
141	Theoretical analysis of the energy levels induced by oxygen vacancies and the doping process (Co, Cu and Zn) on SnO2 (110) surface models. *Computational and Theoretical Chemistry*, **2001**, 541, 69-79		20

140	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		5
139	Quantum-mechanical analysis of the equation of state of anatase TiO2. *Physical Review B*, **2001**, 64,	3.3	63
138	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	2.8	4
137	Transition Structures for d-Ribulose-1,5-bisphosphate Carboxylase/Oxygenase-Catalyzed Oxygenation Chemistry: Role of Carbamylated Lysine in a Model Magnesium Coordination Sphere. *Journal of Physical Chemistry A*, **2001**, 105, 4726-4736	2.8	14
136	A theoretical study of the reaction between cyclopentadiene and protonated imine derivatives: a shift from a concerted to a stepwise molecular mechanism. *Journal of Organic Chemistry*, **2001**, 66, 6151-7	4.2	37
135	Static simulation of bulk and selected surfaces of anatase TiO2. *Surface Science*, **2001**, 490, 116-124	1.8	106
134	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	2.8	8
133	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
132	Topological Analysis of Multiple Metal□Metal Bonds in Dimers of the M2(Formamidinate)4 Type with M = Nb, Mo, Tc, Ru, Rh, and Pd. *Journal of Physical Chemistry A*, **2001**, 105, 9460-9466	2.8	62
131	Molecular structure of the molybdenum oxo-diperoxo compound MoO(O(2))(2)(OPy)(H(2)O): a computational and X-ray study. *Inorganic Chemistry*, **2001**, 40, 6022-5	5.1	28
130	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
129	Quantum Mechanical/Molecular Mechanical Study on the Favorskii Rearrangement in Aqueous Media. *Journal of Physical Chemistry B*, **2001**, 105, 2453-2460	3.4	15
128	A theoretical study on the molecular mechanism for the normal Reimer□Tiemann reaction. *Chemical Physics Letters*, **2000**, 318, 270-275	2.5	7
127	Alternative pathways for the C2□C3 bond cleavage and C2 configuration inversion processes for the Rubisco-catalyzed carboxylation sequence. *Chemical Physics Letters*, **2000**, 318, 361-369	2.5	4
126	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	2.5	15
125	A theoretical study on cytosine tautomers in aqueous media by using continuum models. *Chemical Physics Letters*, **2000**, 317, 437-443	2.5	57
124	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, 3473-7	4.2	18
123	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	3.4	46

122	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	2.3	24
121	Experimental and theoretical study on the piezoelectric behavior of barium doped PZT. *Journal of Materials Science*, **1999**, 34, 3659-3667	4.3	16
120	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
119	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	1.9	27
118	Transition-state structures for describing the enzyme-catalyzed mechanisms of rubisco. *Theoretical Chemistry Accounts*, **1999**, 101, 234-240	1.9	10
117	PM3 study of the domino reaction of nitroalkenes with silyl enol ethers. *Journal of Physical Organic Chemistry*, **1999**, 12, 24-30	2.1	6
116	Theoretical study of the molecular mechanism of the domino pathways for squarate ester sequential reactions. *Journal of Physical Organic Chemistry*, **1999**, 12, 61-68	2.1	2
115	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. *Surface Science*, **1999**, 430, 213-222	1.8	65
114	Theoretical Study of the Mechanisms for the Alkoxyacetic Acids Decomposition. *Journal of Physical Chemistry A*, **1999**, 103, 3935-3943	2.8	33
113	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	4.2	8
112	Structure and Bonding of Chlorine Oxides and Peroxides: ClOx, ClOx-(x= 1 4), and Cl2Ox(x= 1 8). *Journal of Physical Chemistry A*, **1999**, 103, 3078-3088	2.8	69
111	A Theoretical Study of the Molecular Mechanism for the Carboxylation Chemistry in Rubisco. *Journal of Physical Chemistry A*, **1999**, 103, 8725-8732	2.8	14
110	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	4.2	3
109	Theoretical Study of the Molecular Mechanism for the Oxygenation Chemistry in Rubisco. *Journal of Physical Chemistry A*, **1999**, 103, 6009-6016	2.8	13
108	Nonlocal (Pair Site) Reactivity from Second-Order Static Density Response Function: Gas- and Solution-Phase Reactivity of the Acetaldehyde Enolate as a Test Case. *Journal of Physical Chemistry A*, **1999**, 103, 1367-1375	2.8	43
107	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
106	Towards an understanding of the molecular mechanism of the unimolecular decomposition of the N-chloro- amino acids on the ground and excited states surfaces in aqueous medium. *Chemical Physics Letters*, **1998**, 283, 294-300	2.5	8
105	Theoretical study of the structure and stability of NbxOy and NbxOy+ (x=1 ; y=2 , 7, 8) clusters. *Chemical Physics Letters*, **1998**, 287, 620-626	2.5	35

104	A theoretical study on the decomposition mechanism of β-propiolactone and β-butyrolactone. *Chemical Physics Letters*, **1998**, 288, 261-269	2.5	7
103	A theoretical analysis on the intramolecular proton transfer of β-alanine in an aqueous medium. *Chemical Physics Letters*, **1998**, 294, 1-8	2.5	15
102	Molecular mechanism for oxygenation pathway in Rubisco.: Mapping transition structures and intermediates for model compounds of the substrate system. *Chemical Physics Letters*, **1998**, 294, 87-94	2.5	12
101	A PM3 theoretical study of the adsorption and dissociation of water on MgO surfaces. *Computational and Theoretical Chemistry*, **1998**, 426, 199-205		10
100	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		8
99	A theoretical study of the addition of CH3MgCl to chiral β-alkoxy carbonyl compounds. *Computational and Theoretical Chemistry*, **1998**, 426, 263-275		3
98	A density functional theory analysis of the gas and solution phase isomerization reactions of MCN, (M = H, Li, Na) systems. *Computational and Theoretical Chemistry*, **1998**, 426, 277-288		11
97	A PM3 semiempirical study of the molecular mechanism for the Favorskii rearrangement of the β-chlorocyclobutanone. *Computational and Theoretical Chemistry*, **1998**, 426, 299-306		3
96	Theoretical investigation of the abnormal Reimer–Tiemann reaction. *Journal of Physical Organic Chemistry*, **1998**, 11, 670-677	2.1	2
95	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	2.1	28
94	Hydrogen bonding and dissociation effects on the gas phase proton transfer reactions of ozone. *Theoretical Chemistry Accounts*, **1998**, 99, 60-63	1.9	2
93	Theory of non-local (pair site) reactivity from model static-density response functions. *Theoretical Chemistry Accounts*, **1998**, 99, 183-191	1.9	16
92	A theoretical study of the unimolecular decomposition of N-chloro-β-amino acids in aqueous solution. *Chemical Physics*, **1998**, 229, 125-136	2.3	9
91	Toward an Understanding of Molecular Mechanism of Domino Cycloadditions. Density Functional Theory Study of the Reaction between Hexafluorobut-2-yne and N,N'-Dipyrrolylmethane. *Journal of the American Chemical Society*, **1998**, 120, 1617-1618	16.4	59
90	Ab Initio Study of Stereo- and Regioselectivity in the Diels–Alder Reaction between 2-Phenylcyclopentadiene and β-(Methylthio)acrylonitrile. *Journal of Organic Chemistry*, **1997**, 62, 1775-1778	4.2	30
89	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
88	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
87	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 β-Chlorocyclobutanone. *Journal of the American Chemical Society*, **1997**, 119, 1941-1947	16.4	22

86	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		11
85	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		22
84	Piezoelectric behaviour of PZT doped with calcium: a combined experimental and theoretical study. *Journal of Materials Science*, **1997**, 32, 2381-2386	4.3	14
83	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	3.4	5
82	A quantum electronic theory of chemical processes The inverted energy profile case: CH3+ + H2 reaction. *International Journal of Quantum Chemistry*, **1997**, 63, 373-391	2.1	6
81	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	2.1	3
80	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	2.1	4
79	Potential energy surface for the decomposition of mandelic acid. *Chemical Physics Letters*, **1997**, 274, 422-428	2.5	32
78	Transition structures of carbon dioxide fixation, hydration and C2 inversion for a model of Rubisco catalyzed reaction. *Chemical Physics Letters*, **1997**, 278, 291-296	2.5	16
77	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		13
76	Unimolecular Decomposition of the Anionic Form of N-Chloro-glycine. A Theoretical Study. *The Journal of Physical Chemistry*, **1996**, 100, 3561-3568		14
75	A Theoretical Study of Addition of Organomagnesium Reagents to Chiral Alkoxy Carbonyl Compounds. *Journal of Organic Chemistry*, **1996**, 61, 3467-3475	4.2	23
74	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	4.2	20
73	A comparative QCISD(T), DFT and MCSCF study of the unimolecular, decomposition of the N-chloro-glycine anion in gas phase. *Theoretica Chimica Acta*, **1996**, 94, 247-256		5
72	Transition structure for hydride transfer from cyclopropene to azirinium cation. *Computational and Theoretical Chemistry*, **1996**, 363, 257-261		1
71	CO interaction with ZnO surfaces: an MNDO, AM1 and PM3 theoretical study with large cluster models. *Computational and Theoretical Chemistry*, **1996**, 363, 249-256		13
70	Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study. *Chemical Physics*, **1996**, 206, 57-61	2.3	14
69	Transition structures for hydride transfer reactions in vacuo and their role in enzyme catalysis. *Computational and Theoretical Chemistry*, **1996**, 371, 299-312		7

68	Theoretical study of substituent effects in the unimolecular decomposition of N-chloro-α-amino acid anions. Analysis of transition structure and molecular reaction mechanism. *Journal of Physical Organic Chemistry*, **1996**, 9, 371-380	2.1	9
67	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	2.1	3
66	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	2.1	11
65	H2O and H2 interaction with ZnO surfaces: A MNDO, AM1, and PM3 theoretical study with large cluster models. *International Journal of Quantum Chemistry*, **1996**, 57, 861-870	2.1	41
64	On Transition Structures for Hydride Transfer Step: A Theoretical Study of the Reaction Catalyzed by Dihydrofolate Reductase Enzyme. *Bioorganic Chemistry*, **1996**, 24, 10-18	5.1	30
63	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. *Tetrahedron*, **1996**, 52, 10693-10704	2.4	30
62	The tandem Diels-Alder reaction of dimethyl acetylenedicarboxylate to bicyclopentadiene. A theoretical study of the molecular mechanisms. *Tetrahedron Letters*, **1996**, 37, 7573-7576	2	8
61	An ab initio perturbed ion study of structural properties of TiO2, SnO2 and GeO2 rutile lattices. *Chemical Physics*, **1996**, 212, 381-391	2.3	24
60	Simulation of ionic crystals: calculation of Madelung potentials for stabilized zirconia. *Journal of Materials Science*, **1995**, 30, 4852-4856	4.3	1
59	MgAl2O4 spinel crystal structure. An ab initio perturbed ion study. *International Journal of Quantum Chemistry*, **1995**, 56, 685-694	2.1	3
58	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		25
57	Ionic structures as intercalation compound host lattices. An ab initio perturbed ion study on lattice stretching. *Computational and Theoretical Chemistry*, **1995**, 330, 313-317		2
56	Ab initio perturbed ion calculations on Ni2+□KZnF3 and Ni2+ □KMgF3. A structural study. *Computational and Theoretical Chemistry*, **1995**, 330, 319-323		1
55	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
54	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		24
53	Theoretical study of cluster models and molecular hydrogen interaction with SnO2 [110] surface. *Computational and Theoretical Chemistry*, **1995**, 335, 167-174		15
52	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		19
51	Transition structures in vacuo and the theory of enzyme catalysis. RubiscoꞱs catalytic mechanism: a paradigmatic case?. *Computational and Theoretical Chemistry*, **1995**, 342, 131-140		19

50	Garnet Crystal Structures. An ab Initio Perturbed Ion Study. *The Journal of Physical Chemistry*, **1995**, 99, 6493-6501		7
49	Pseudopotential Periodic Hartree-Fock study of K8In11 and Rb8In11 Systems. *The Journal of Physical Chemistry*, **1995**, 99, 12483-12487		10
48	A theoretical study of the molecular mechanism for the oxidation of methanol by PQQ. *Journal of the American Chemical Society*, **1995**, 117, 8807-8815	16.4	22
47	An ab Initio Perturbed Ion Study of the BaLiF3 and BaLiH3 Inverted Perovskite Structures. *The Journal of Physical Chemistry*, **1995**, 99, 8082-8090		3
46	Transition state structures for the molecular mechanism of lactate dehydrogenase enzyme. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 1551-1558		9
45	Theoretical study of lattice stability and selective doping effects of V4+ and Tb4+ in the ZrGeO4 lattice. *Chemical Physics Letters*, **1995**, 236, 521-531	2.5	2
44	An Ab initio perturbed ion study of pyrope garnet structure. *Journal of Physics and Chemistry of Solids*, **1995**, 56, 901-906	3.9	4
43	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		14
42	An ab initio perturbed ion study of bulk ceria. *Chemical Physics Letters*, **1994**, 221, 249-254	2.5	6
41	Quantum Chemical Studies of Pyrroloquinoline Quinone: PM3 Pathways for Methanol Oxidation. *Bioorganic Chemistry*, **1994**, 22, 58-71	5.1	5
40	Quantum chemical study of the adsorption of water on zinc oxide surface. *Computational and Theoretical Chemistry*, **1994**, 303, 19-24		17
39	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		8
38	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		38
37	Theoretical kinetic isotope effects for the hydride-transfer step in lactate dehydrogenase. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 1703-1707		31
36	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
35	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		12
34	A theoretical study of the addition mechanism of carbon dioxide to methylamine. Modelling CO2Biotin fixation. *Journal of the Chemical Society Perkin Transactions II*, **1993**, 521-523		10
33	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 Rubiscols substrate. *The Journal of Physical Chemistry*, **1993**, 97, 7888-7893		26

32	A PM3 Quantum Chemical Study of the Pyruvate Reduction Mechanism Catalyzed by Lactate Dehydrogenase. *Bioorganic Chemistry*, **1993**, 21, 260-274	5.1	11
31	V4+ doping into SiO2, ZrO2 and ZrSiO4 structures. An ab initio perturbed ion study. *International Journal of Quantum Chemistry*, **1993**, 48, 175-186	2.1	3
30	ZnO clusters models: An AM1 and MNDO study. *International Journal of Quantum Chemistry*, **1993**, 48, 643-653	2.1	11
29	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		21
28	True and apparent oxygen permeabilities of contact lenses. *Optometry and Vision Science*, **1992**, 69, 685-90	2.1	18
27	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		23
26	Amidine decomposition mechanism. A theoretical study. *Computational and Theoretical Chemistry*, **1992**, 254, 465-472		16
25	Straining the double bond in 1,2-dihydroxyethylene. A simple theoretical model for the enediol moiety in Rubiscols substrate and analogs. *Chemical Physics Letters*, **1992**, 198, 515-520	2.5	23
24	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	2.5	26
23	Electronic aspects of LADH catalytic mechanism. *International Journal of Quantum Chemistry*, **1991**, 39, 767-786	2.1	40
22	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	2.1	5
21	Theoretical studies of substituent effects on stationary structures of amidine decomposition. *Journal of the Chemical Society Perkin Transactions II*, **1991**, 539-542		1
20	Theoretical rotational constants of MeCnN species. *Chemical Physics Letters*, **1990**, 166, 54-56	2.5	8
19	Calculation of the relative basicities of methylamines in solution. *Chemical Physics Letters*, **1990**, 169, 297-300	2.5	12
18	Theoretical study of stationary structures of acetamidine unimolecular decomposition. *Chemical Physics Letters*, **1990**, 169, 509-512	2.5	8
17	HCnN: The largest molecules in the interstellar medium. *Journal of Chemical Education*, **1990**, 67, 905	2.4	16
16	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	16.4	34
15	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

14	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
13	Electronic aspects of the hydride transfer mechanism. *Computational and Theoretical Chemistry*, **1988**, 167, 395-412		18
12	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		6
11	Theoretical studies of acetylenic alcohols rearrangement mechanism: Ab initio calculations of the unimolecular rate limiting step. *Computational and Theoretical Chemistry*, **1986**, 138, 171-177		4
10	Catalytic role of copper(I) ion on the propargylic transposition. A theoretical study. *The Journal of Physical Chemistry*, **1985**, 89, 4769-4773		6
9	Linear bending in propynyl cation, allene, and propyne systems: do they have flexible structures? an ab initio 4 31 + G molecular orbital study. *Journal of the Chemical Society Perkin Transactions II*, **1985**, 363-366		3
8	Electronic aspects of the hydride transfer mechanism. Ab initio analytical gradient studies of the cyclopropenyl-cation/lithium hydride model reactant system. *Journal of Chemical Physics*, **1985**, 83, 4673-4682	3.0	24
7	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	2.5	1
6	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
5	Quantum-chemical studies of the energy hypersurface for the Meyer–Schuster rearrangement STO-3G calculation of minimum-energy paths. Intermolecular mechanism. *Chemical Physics Letters*, **1983**, 94, 193-197	2.5	8
4	A theoretical study of the intramolecular solvolytic mechanism of the Meyer–Schuster reaction. MINDO/3 and CNDO/2 calculations of minimum energy paths. *Computational and Theoretical Chemistry*, **1983**, 105, 49-54		7
3	A quantum chemical study of protonated intermediates in Rupe and Meyer-Schuster rearrangement mechanisms. *Computational and Theoretical Chemistry*, **1983**, 105, 307-314		8
2	Reading at exposed surfaces: theoretical insights into photocatalytic activity of ZnWO41, 1005		11
1	Ag nanoparticles-based antimicrobial polycotton fabrics to prevent the transmission and spread of SARS-CoV-2		16