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694	Structural, spectroscopic, FMOs, and non-linear optical properties exploration of three thiacaix(4)arenes derivatives. <b>2022</b> , 15, 103656	4
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692	Synthesis, spectral characterization, chemical reactivity and anticancer behaviors of some novel hydrazone derivatives: Experimental and theoretical insights. <b>2022</b> , 1253, 132224	3
691	CdSe/ZnS quantum dots capped with oleic acid and L-glutathione: Structural properties and application in detection of Hg2+. <b>2022</b> , 1254, 132293	1
690	Cyanomethylation of 2,3,4,9-tetrahydro-1H-carbazol-1-one based on using two different reagents: Antioxidant activity and DFT studies. <b>2022</b> , 1253, 132262	
689	Synthesis and investigation of anti-COVID19 ability of ferrocene Schiff base derivatives by quantum chemical and molecular docking <b>2022</b> , 1253, 132242	1
688	Adsorptive Complexation and Isotope Separation of Gadolinium Ion with Macrocyclic Crown Ether Embedded Polymeric Resin: Theory Guided Experiments.	
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684	Ternary adsorption of Auramine-O, Rhodamine 6G, and Brilliant Green onto Arapaima gigas scales hydroxyapatite: Adsorption mechanism investigation using CCD and DFT studies. <b>2022</b> , 31, e00391	0
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677	Probing the interaction of new and biologically active Pd(II) complex with DNA/BSA via joint experimental and computational studies along with thermodynamic, NLO, FMO and NBO analysis <b>2022</b> , 35, 245	1
676	Evaluation of the mechanism, regio-, and diastereoselectivity of aza-DielsAlder reactions of 2H-azirine under a Lewis acid catalyst. <b>2022</b> , 33, 445	
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671	DFT Studies and Quantum Chemical Calculations of Benzoyl Thiourea Derivatives Linked with Morpholine and Piperidine for the Evaluation of Antifungal Activity. <b>2022</b> , 12,	
670	Comparison of green bio-based cerium/alginate vs. copper/alginate beads: a study of vibrational and thermal properties using experimental and theoretical methods <b>2022</b> , 28, 37	
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667	Electronic Properties of Aldehyde Complexes Using DFT for Electrooptical Activity. 1048, 212-220	
666	Design of dyes for energy transformation: From the interaction with biological systems to application in solar cells. <b>2022</b> , 79-114	
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664	In silico evaluation of molecular interactions between macrocyclic inhibitors with the HCV NS3 protease. Docking and identification of antiviral pharmacophore site <b>2022</b> , 1-14	1
663	New 1,2,3-Triazoles from (R)-Carvone: Synthesis, DFT Mechanistic Study and In Vitro Cytotoxic Evaluation <b>2022</b> , 27,	6
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656	Olefin Metathesis Catalyzed by a Hoveyda-Grubbs-like Complex Chelated to Bis(2-mercaptoimidazolyl) Methane: A Predictive DFT Study <b>2022</b> ,	О
655	Investigation of Corrosion Inhibition Potentials of Some Aminopyridine Schiff Bases Using Density Functional Theory and Monte Carlo Simulation. <b>2022</b> , 5, 319	4
654	Exploring Molecular and Electronic Property Predictions of Reduced Graphene Oxide Nanoflakes via Density Functional Theory <b>2022</b> , 7, 3872-3880	1
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648	Do nitrate ions preferentially bind to Ln/An ion in nuclear waste treatment? [Answers from DFT calculations. <b>2022</b> , 215, 115691	2
647	Kaya's composite descriptor and Maximum Composite Hardness Rule for chemical reactions. <b>2022</b> , 99, 100364	O
646	Predicting the reactivity of unsaturated molecules to methyl radical addition using a radical two-parameter general-purpose reactivity indicator. <b>2022</b> , 791, 139333	0
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642	Effect of #adiations on the optoelectrical parameters of coumarin-poly vinyl alcohol composite thin films. <b>2022</b> , 193, 109973	О
641	Quantum computational, spectroscopic investigations on N-(2-((2-chloro-4,5-dicyanophenyl)amino)ethyl)-4-methylbenzenesulfonamide by DFT/TD-DFT with different solvents, molecular docking and drug-likeness researches. <b>2022</b> , 638, 128311	35
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639	Synthesis, spectral, structural and antimicrobial activities of Ethyl-4-{[-(1-(2-(4-nitrobenzoyl)hydrazono)ethyl]}-3,5-dimethyl-1H-pyrrole-2-carboxylate. <b>2022</b> , 1255, 132405	
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637	Wearable Light Sensors Based on Unique Features of a Natural Biochrome 2022,	3
636	Quantitative structure-activity relationship study of skin sensitization of Michael acceptors based on quantum chemical descriptors. <b>2022</b> ,	
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634	Structural changes and photocatalytic aspects into anatase network after doping with cerium: comprehensive study via radial distribution functions, electron density maps and molecular hardness. <b>2022</b> , 428, 113855	
633	Synthesis of thiophene derivatives: Substituent effect, Antioxidant activity, Cyclic voltammetry, Molecular Docking, DFT, and TD-DFT Calculations. <b>2022</b> , 1257, 132607	1

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627	Synthesis, vibrational Depictions, IRI interpretations and docking research on coordination metal complex Diaqua aspartato zinc (II) monohydrate using DFT approach. <b>2022</b> , 351, 118687	1
626	Highly efficient and selective removal of Sr2+ from aqueous solutions using ammoniated zirconium phosphate. <b>2022</b> , 10, 107333	2
625	Synthesis, crystallographic study, molecular docking, ADMET, DFT and biological evaluation of new series of aurone derivatives as anti-leishmanial agents. <b>2022</b> , 1256, 132528	3
624	Synthesis, structural, computational, and antiproliferative activity studies of new steroidal tetrazole derivatives. <b>2022</b> , 1256, 132577	О
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620	Unveiling the intramolecular $[3 + 2]$ cycloaddition reactions of C,N-disubstituted nitrones from the molecular electron density theory perspective.	O
619	Thiophene derivatives as corrosion inhibitors for 2024-T3 aluminum alloy in hydrochloric acid medium <b>2022</b> , 12, 10321-10335	1
618	Computational Investigation on Structural and Reactive Sites (HOMO-LUMO, MEP, NBO, NPA, ELF, LOL, RDG) Identification, Pharmacokinetic (ADME) Properties and Molecular Docking Investigation of (E)-4-((4-chlorobenzylidene) amino) Benzene Sulfonamide Compound. <b>2022</b> , 12, 58-76	3
617	Ultrasound-Assisted Micro-Channel Extraction of Magnesium from Wet-Process Phosphoric Acid. <b>2022</b> , 29, 9-19	
616	Lithium Selectivity of Crown Ethers: The Effect of Heteroatoms and Cavity Size.	
615	Orthogonal reactivity and interface-driven selectivity during cation exchange of heterostructured metal sulfide nanorods <b>2022</b> ,	

614	Spectroscopic Identification, Structural Features and Molecular Docking Studies on 5-(4-Propoxybenzylidene)-2-[3-(4-chlorophenyl)-5-[4(propan-2-yl) phenyl-4,5-dihydro-1H-pyrazol-1-yl]-1,3-thiazol-4(5H)-one using Pim-1 Kinase Cancer Protein. <b>2022</b> , 34, 857-870	
613	Electrochemical behaviour of 2-hydroxybenzophenones and related molecules. <b>2022</b> , 4, 100332	1
612	An experimental and computational study of new spiro-barbituric acid pyrazoline scaffolds: restricted rotation vs. annular tautomerism.	2
611	SYNTHESIS, CRYSTAL STRUCTURE, AND DFT STUDY OF N-(2-FLUORO-4-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXIN-2-YL)PHENYL)- 3-METHYL-BUTANAMIDE. <b>2022</b> , 63, 100-113	
610	PM3 Method based QSAR Study of the Derivatives of Thiadiazole and Quinoxaline for Antiepileptic Activity using Quantum Mechanical and Energy Descriptors. <b>2022</b> , 7, 111-122	
609	A thermodynamic criterion for the choice of flux and its validity in NaBO2-fluxed BaB2O4 crystal growth.	
608	SYNTHESIS, CRYSTAL STRUCTURE, DFT CALCULATIONS AND VIBRATIONAL PROPERTIES OF METHYL(tert-BUTOXYCARBONYL)-L- TYROSINATE AND METHYL(2,2,2-TRIFLUOROACETYL)-L-TYROSINATE. <b>2022</b> , 63, 114-124	
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606	Exploration of plant-derived natural polyphenols toward COVID-19 main protease inhibitors: DFT, molecular docking approach, and molecular dynamics simulations <b>2022</b> , 12, 5357-5368	1
605	Density Functional Tight Binding Calculations for Probing Electronic-Excited States of Large Systems. <b>2022</b> , 45-79	
604	Molecular Structural, Hydrogen Bonding Interactions, and Chemical Reactivity Studies of Ezetimibe-L-Proline Cocrystal Using Spectroscopic and Quantum Chemical Approach <b>2022</b> , 10, 848014	О
603	A quest for substituent effects on novel diamino(phosphino)phosphinidenes using density functional theory method.	
602	From the Electron Density Gradient to the Quantitative Reactivity Indicators: Local Softness and the Fukui Function <b>2022</b> , 7, 7745-7758	1
601	Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability <b>2022</b> , 156, 084104	5
600	Hybrid Synthetic and Computational Study of an Optimized, Solvent-Free Approach to Curcuminoids <b>2022</b> , 7, 7257-7277	О
599	Structural, Electronic, Vibrational and Pharmacological Investigations of Highly Functionalized Diarylmethane Molecules Using DFT Calculations, Molecular Dynamics and Molecular Docking. 1-19	1
598	Antiradical properties of curcumin, caffeic acid phenethyl ester, and chicoric acid: a DFT study <b>2022</b> , 28, 68	О
597	Fischer and Schrock carbene complexes in the light of global and local electrophilicity-based descriptors.	

596	Computational Investigation of Chemisorption of Thiophosgene on Co@B $$$ _{8}^{-}\$. <b>2022</b> , 96, 267-272	
595	Molecular Structure, Experimental and Theoretical Vibrational Spectroscopy, (HOMO-LUMO, NBO) Investigation, (RDG, AIM) Analysis, (MEP, NLO) Study and Molecular Docking of Ethyl-2-{[4-Ethyl-5-(Quinolin-8-yloxyMethyl)-4H-1,2,4-Triazol-3-yl] Sulfanyl} Acetate. 1-25	3
594	Probing the biomolecular (DNA/BSA) interaction by new Pd(II) complex via in-depth experimental and computational perspectives: synthesis, characterization, cytotoxicity, and DFT approach. 1	1
593	Spectroscopic, Solvation Effects and MD Simulation of an Adamantane-Carbohydrazide Derivative, a Potential Antiviral Agent. 1-15	1
592	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. <b>2022</b> , 137, 1	2
591	Organic Compounds as Corrosion Inhibitors for Carbon Steel in HCl Solution: A Comprehensive Review <b>2022</b> , 15,	4
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589	A novel chemo-phenotypic method identifies mixtures of salpn, vitamin D3, and pesticides involved in the development of colorectal and pancreatic cancer <b>2022</b> , 233, 113330	Ο
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587	Kernel charge equilibration: efficient and accurate prediction of molecular dipole moments with a machine-learning enhanced electron density model. <b>2022</b> , 3, 015032	O
586	Unveiling Role of Metals in Mononuclear Metal-Complexes for Chemodosimetric Detection of S 2 from aqueous medium: Experimental and DFT Corroboration with Real-Field Application. <b>2022</b> , 7,	0
585	Cyanopropyl functionalized benzimidazolium salts and their silver N-heterocyclic carbene complexes: Synthesis, antimicrobial activity, and theoretical analysis <b>2022</b> , e2200041	O
584	Novel Sulfur-Containing Porous Organic Polymer as a Nanotrap for Rapid Removal of Mercury(II) from Environmental Waters. <b>2022</b> , 61, 3694-3703	0
583	Synthesis of the nickel(II) complexes bearing tetradentate thiosemicarbazone through Michael addition of n-alcohols. Experimental, theoretical characterization and antioxidant properties. 1	
582	Molecular docking, X-ray crystallography, Hirshfeld surface and computational studies of N-((2,3-dichlorophenyl)(ethoxy)methyl)-2-methoxy-4-nitrobenzenamine. 1-29	
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580	Simple Models of Charge-Transfer Reactivity. <b>2022</b> , 12,	
579	Reactivity and a Charge-Transfer Model Analysis in Aminopolycarboxylic-Metal Complexes <b>2022</b> ,	

578	Alterations to the broad-spectrum formin inhibitor SMIFH2 improve potency.	O
577	The effects of heteroatom substituents on structure, stability, and electronic properties of remote N -heterocyclic germylenes (rNHGes), at DFT.	
576	[Tb4(OH)4]-Cuboid Complex Dianion Stabilized with Six Carboxylate Bridges and Four Diketonate Caps. <b>2022</b> , 12, 402	
575	Experimental and Quantum Chemical Studies of Nicotinamide-Oxalic Acid Salt: Hydrogen Bonding, AIM and NBO Analysis <b>2022</b> , 10, 855132	1
574	Model of BN Response under External Electric Field: Geometry, Electronic Properties, Reaction Activity <b>2022</b> , 27,	О
573	Deep oxidative desulfurization via rGO-immobilized tin oxide nanocatalyst: Experimental and theoretical perspectives. <b>2022</b> , 33, 103499	1
572	Quantum Computational Investigation of ()-1-(4-methoxyphenyl)-5-methyl-'-(3-phenoxybenzylidene)-1-1,2,3-triazole-4-carbohydrazide <b>2022</b> , 27,	12
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570	Mechanistic Investigations of the Synthesis of Lactic Acid from Glycerol Catalyzed by an Iridium NHC Complex. <b>2022</b> , 10, 626	0
569	Ocimum tenuiflorum L mediated green synthesis of silver and selenium nanoparticles: antioxidant activity, cytotoxicity and density functional theory studies. <b>2022</b> , 13, 015015	O
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559	Molecular insights into the encapsulation of fluorouracil molecule inside the single-walled carbon nanotubes. <b>2022</b> , 124, 108900	O
558	Exploring the maximum Fukui function sites with the frontier-controlled soft-soft reactions using 1,3-dipolar cycloaddition reactions of nitrilium betaines <b>2022</b> , 28, 116	0
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552	DFT, MD simulations and experimental analysis of adsorptive complexation and isotope separation of gadolinium ion with macrocyclic crown ether embedded polymeric resin. <b>2022</b> , 289, 120709	0
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550	Spectroscopic, physicochemical, and pharmacokinetic analysis of ∃,⊞myrin mixture obtained from Protium heptaphyllum (Aubl.) Marchand resin. <b>2022</b> , 1256, 132551	1
549	Vibrational spectra and molecular docking studies of bergapten isolated from Melicopedenhamii leaves as anti-breast cancer agents. <b>2022</b> , 1258, 132656	O
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547	Pursuing efficient systems for glucose transformation to levulinic acid: Homogeneous vs. heterogeneous catalysts and the effect of their co-action. <b>2022</b> , 318, 123712	1
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533	An Unusual Pair: Facile Formation and In Vivo Validation of Robust Sc-18F Ternary Complexes for Molecular Imaging. <b>2021</b> ,	1
532	Discovery Potent of Thiazolidinedione Derivatives as Antioxidant, <code>\pi-Amylase Inhibitor</code> , and Antidiabetic Agent <b>2021</b> , 10,	3
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479 47 <sup>8</sup>			О
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467	Comparative efficiency of polycyclic aromatic hydrocarbon removal by novel graphene oxide composites prepared from conventional and green synthesis. <b>2022</b> , 132244	2
466	Facile Preparation of Millimeter-Sized Sodium Alginate-Silica Composite Spheres for Highly Selective Adsorption of Heavy Metal Ions. <b>2022</b> , 7,	O
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464	New graphene oxide-safranin modified@polyacrylonitrile membranes for removal of emerging contaminants: The role of chemical and morphological features. <b>2022</b> , 137176	О
463	Guerbet Coupling of Methanol Catalysed by Titanium Clusters. <b>2022</b> , 139719	
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450	Synthesis of Cinnamoyl-Amino Acid Ester Derivatives and Structure-Activity Relationship Based on Thermal Stability, Dielectric, and Theoretical Analysis. <b>2022</b> , 7,	0
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446	The inhibition performance of diaminoalkanes functionalized GOs against carbon steel corrosion in 15% HCl environment. <b>2022</b> , 137402	1
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435	Computational Methods of Corrosion Inhibition Assessment. 87-109	O

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433	A Predictive Chemistry DFT Study of the N2O Functionalization for the Preparation of Triazolopyridine and Triazoloquinoline Scaffolds.	2
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422	The effect of anchoring group on the performances of metal-free phthalocyanine and metallophthalocyanine dye/titanium dioxide interface for dye-sensitized solar cells. <b>2022</b> , 102089	1
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406	Removal of neonicotinoid pesticides by adsorption on modified Tenebrio molitor frass biochar: Kinetics and mechanism. <b>2022</b> , 297, 121506	0
405	Structure and optical properties of new nitro-derivatives of 2-N-alkiloamino-picoline N-oxide isomers. <b>2022</b> , 1265, 133372	
404	Synthesis, crystal structure and ATR-FTIR, FT-Raman and UVII is spectroscopic analysis of dihydrochalcone (3R)-3-(4-chlorophenyl)-3-hydroxy-1-(2-hydroxyphenyl)propan-1-one. <b>2022</b> , 1266, 133516	1
403	Development, synthesis, computational and in silico investigations of Pd(II)-catalyzed aryl fluorinated and hydroxylated sulfonamides. <b>2022</b> , 1266, 133481	O
402	Design, Synthesis, Biological evaluation of Isonicotinoyl-pyrazolyl-coumarin derivatives and computational study. <b>2022</b> , 1265, 133487	
401	Spectroscopic, electronic structure, molecular docking, and molecular dynamics simulation study of 7-Trifluoromethyl-1H-indole-2-carboxylic acid as an aromatase inhibitor. <b>2022</b> , 280, 121530	
400	Importance of ligand design in lanthanide azamacrocyclic complexes relevant to biomedical applications. <b>2022</b> ,	
399	Rational design of small molecule hole-transporting materials with linear Ebridge for highly efficient perovskite solar cells.	

 $\,$  Janus Dione Derivatives: Novel High-Mobility Hole Transport Materials for Perovskite Solar Cells.

397	Conceptual Density Functional Theory under Pressure: Part I. XP-PCM Method Applied to Atoms.	O
396	Wide Nematogenic Azomethine/Ester Liquid Crystals Based on New Biphenyl Derivatives: Mesomorphic and Computational Studies. <b>2022</b> , 27, 4150	5
395	Synthesis, in vitro cholinesterase inhibition, molecular docking, DFT and ADME studies of novel 1,3,4-oxadiazole 2-thiol derivatives.	1
394	On the Prediction of Lattice Energy with the Fukui Potential: Some Supports on Hardness Maximization in Inorganic Solids. <b>2022</b> , 126, 4507-4516	1
393	Surface Reactivity of Cementitious Crystals Alite and Belite. <b>2022</b> , 126, 11265-11276	
392	Insights into the mechanism and stereoselectivity of the [3+2] cycloaddition reaction between N-methyl-C-(4-hydroxylphenyl) nitrone and maleic anhydride with a molecular electron density theory perspective. <b>2022</b> , 141,	0
391	Bir Florlu Aminoimidazolin Olan Midaflur'un Kar⊞la⊞rmal⊞ Kuantum Kimyasal Analizi.	
390	Theoretical investigation of the titaniumBitrogen heterofullerenes evolved from the smallest fullerene. <b>2022</b> , 108269	0
389	Synthesis, crystal structure, DFT calculations and vibrational properties of 1-(2-bromo-4-(dimethylamino)phenyl)-4-(2-chlorobenzyl)-[1,2,4]triazolo[4,3-a]quinazolin-5(4H)-one. 1-12	
388	A systematic computational study of acridine derivatives through conceptual density functional theory.	O
387	DFT evaluation of structural, electronic and variation properties for complex carbohydrates with biological interest. 1-9	
386	DFT study of stability and electronic properties of cyclic tetramer involving dinucleobase monomers, comprising acetylene central block substituted at both edges with guanine and cytosine nucleobases.	
385	Estimating structure, stability, and electronic properties on halogenated derivatives of 2-germabicyclo[1.1.1.]pentane-2-ylidenes at density functional theory. <b>2022</b> , 28,	O
384	Silicon Carbide Based Nanotubes as a Sensing Material for Gaseous H2SiCl2.	1
383	Development of a Multifunctional Aggregation-Induced Emission-Active White Light-Emissive Organic Sensor: A Combined Theoretical and Experimental Approach.	
382	Adsorptive removal of toxic malachite green from its aqueous solution by Bambusa Vulgaris Leaves and its acid-treated form: DFT, MPR and GA modeling. <b>2022</b> , 119841	1
381	Synthesis, Molecular Structure and Theoretical Calculations of 4-Aminopyridinium Benzoate. <b>2022</b> ,	O

 $_{3}8\mathrm{o}$   $\,$  Synthesis and characterization of cobalt SCS pincer complexes.

379	Synthesis, <code>\B-Glucosidase Inhibition</code> , Anticancer, DFT and Molecular Docking Investigations of Pyrazole Hydrazone Derivatives. 1-20	2
378	Experimental and theoretical insights into two fluorine-containing imidazoline Schiff base inhibitors for carbon steels in hydrochloric acid solution. <b>2022</b> , 133737	1
377	The Interaction of Deep Eutectic Solvents with Pristine Carbon Nanotubes and Their Associated Defects: A Density Functional Theory Study. <b>2022</b> , 119855	O
376	Indium and Tin Doping of Zinc Oxide Film by Cation Exchange and its Application to Low-Temperature Thin-Film Transistors. 2200190	О
375	Density functional theory studies of polypyrrole and polypyrrole derivatives; substituent effect on the optical and electronic properties. <b>2022</b> , 255, 125127	O
374	Experimental, DFT and Theoretical Corrosion Study for 4-(((4-ethyl-5-(thiophen-2-yl)-4H-1,2,4-triazole-3-yl)thio)methyl)-7,8-dimethyl-2H-chromen-2-one. <b>2022</b> , 15, 104088	1
373	Experimental and DFT theoretical study for understanding the adsorption mechanism of toxic dye onto innovative material Fb-HAp based on fishbone powder. <b>2022</b> , 362, 119739	O
372	The role of herbal plants in the inhibition of SARS-CoV-2 main protease: A computational approach. <b>2022</b> , 99, 100640	
371	Synthetic approach to achieve halo imine units: Solid-state assembly, DFT based electronic and non linear optical behavior. <b>2022</b> , 803, 139843	6
370	Vanillin based colorimetric and fluorometric chemosensor for detection of Cu(II) ion: DFT calculation, DNA / BSA interaction and molecular docking studies. <b>2022</b> , 143, 109716	1
369	Iron oxide nanoparticles loaded smart hybrid hydrogel for anti-inflammatory drug delivery: Preparation and characterizations. <b>2022</b> , 650, 129631	5
368	The electronic structures and nonlinear optical properties of Alkali and Alkali earth metal atoms doped C6H6Cl6: A density functional theoretical study. <b>2022</b> , 116, 108263	
367	Physicochemical properties calculated using DFT method and changes of 5-methyluridine hemihydrate crystals at high temperatures. <b>2022</b> , 281, 121594	
366	Molecular interactions from the density functional theory for chemical reactivity: Interaction chemical potential, hardness, and reactivity principles. 10,	1
365	Layered potassium calcium phosphate with multiple exchangeable cations for Sr(II) and Co(II) removal from water. <b>2022</b> , 121789	1
364	Synthesis, Characterization, Molecular Docking and Molecular Dynamics Simulations of Benzamide Derivatives as Potential Anti-Ovarian Cancer Agents. <b>2022</b> , 133785	10
363	Spectral characterization, solvation effects on topological aspects, and biological attributes of Fmoc-L-glutamic acid 5-tert-butyl ester: An effective reagent in anticancer evaluations. <b>2022</b> , 133793	1

362	Spectroscopic Investigation and Density Functional Theory prediction of First and Second order Hyperpolarizabilities of 1-(4-Bromophenyl)-3-(2,4-dichlorophenyl)-prop-2-en-1-one. <b>2022</b> , 133807	2
361	Study by DFT of the functionalization of amylose/amylopectin with glycerin monoacetate: Characterization by FTIR, electronic and adsorption properties. <b>2022</b> , 1269, 133761	Ο
360	Imidazole and nitroimidazole derivatives as NADH -fumarate reductase inhibitors: Density functional theory studies, homology modeling, and molecular docking. <b>2022</b> , 43, 1573-1595	Ο
359	Synthesis crystal structure, and DFT study of ethyl 2-ethylimidazo[1,2-a]pyridine-3-carboxylate. 1-10	
358	Decomposition of dinitrosyl iron complex with thioformaldehyde ligands in water: reaction mechanisms and the role of chemical hardness of ligands. <b>2022</b> , 32, 457-459	
357	Adsorption of Pesticides, Antibiotics and Microcystin-LR by Graphene and Hexagonal Boron Nitride Nano-Systems: A Semiempirical PM7 and Theoretical HSAB Study. <b>2022</b> , 12, 1068	Ο
356	A study of 5-lipoxygenase inhibitors invoking DFT-based descriptor nucleophilicity index. <b>2022</b> , 153, 651-656	
355	Palladium-Doped Single-Walled Carbon Nanotubes as a New Adsorbent for Detecting and Trapping Volatile Organic Compounds: A First Principle Study. <b>2022</b> , 12, 2572	O
354	Unveiling the Chemistry of Higher-Order Cycloaddition Reactions within the Molecular Electron Density Theory. <b>2022</b> , 4, 735-752	1
353	Hydrogen storage capacity of Be 2 (NLi) 2 cluster with ultra-short berylliumBeryllium distance.	
352	XPS photoelectron lines, satellite structures and Wagner plot of Cu(II)	0
351	Synthesis, Characterization, and DFT-Based Electronic and Nonlinear Optical Properties of Methyl 1-(arylsulfonyl)-2-aryl-1H-benzo[d]imidazole-6-carboxylates.	
350	Electronegativity Equilibration. <b>2022</b> , 126, 5472-5482	
349	A combined study on structures and vibrational spectra of the antiviral rimantadine using SQMFF and DFT calculations. <b>2022</b> , 8, e10102	O
348	Incorporating Comonomers into Polymeric Phosphate Ligands Can Tune the Affinity and Capacity for Rare Earth Element, La.	
347	New findings on ligand series used as SARS-CoV-2 virus inhibitors within the frameworks of molecular docking, molecular quantum similarity and chemical reactivity indices. 11, 914	
346	High capacity reversible hydrogen storage in Si substituted and Li decorated C 20 fullerene: Acumen from density functional theory simulations.	1
345	External fields in conceptual density functional theory.	O

344	Structural and vibrational investigation of CisII rans isomers of potent insecticide allethrin. <b>2022</b> , 28,	
343	Physical, chemical and antibacterial properties of 1-methyl-3-(4-vinylbenzyl) imidazol-3-ium chloride ionic liquid: Experimental and ab-initio analysis. <b>2022</b> , 133955	О
342	Exploring flexibility, intermolecular interactions and ADMET profiles of anti-influenza agent isorhapontigenin: A quantum chemical and molecular docking study. <b>2022</b> , 8, e10122	О
341	Derivatives of [P4-VP] 2% DVB as corrosion inhibitors for St-37 in 1´M H2SO4: an experimental and theoretical investigations.	
340	DFT rationalization of metal-catalyst-controlled coupling of carbazole with diazo-naphthalen-2(1H)-one. <b>2022</b> , 529, 112574	
339	AIEgens-NLOphores coumarin-triphenylamine chalcone derivatives: Synthesis, photophysical properties and DFT computational study. <b>2022</b> , 134009	Ο
338	Janus dione derivatives: Novel high-mobility hole transport materials for perovskite solar cells. <b>2022</b> , 32, 104090	
337	Hardness of Molecules and Bandgap of Solids from a Generalized Gradient Approximation Exchange Energy Functional.	
336	Polyaniline Plastic Nanocomposite as Multi-Functional Nanomaterial. 2022, 7,	О
335	Reversible hydrogen storage capacity of Li and Sc doped novel C 8 N 8 cage: Insights from density functional theory.	1
334	Alterations to the broad-spectrum formin inhibitor SMIFH2 modulate potency but not specificity. <b>2022</b> , 12,	О
333	Highly efficient CO2 conversion on a robust metal-organic framework Cu(I)-MFU-4l: Prediction and mechanistic understanding from DFT calculations. <b>2022</b> , 63, 102148	Ο
332	Electronic properties and chemical reactivity of biogenic amine neurotransmitters in gas and solution phase: A DFT study. <b>2022</b> , 1215, 113841	
331	Putrescine adsorption on pristine and Cu-decorated B12N12 nanocages: A density functional theory study. <b>2022</b> , 1215, 113836	O
330	New insights on the adsorption of CI-Reactive Red 141 dye using activated carbon prepared from the ZnCl2-treated waste cotton fibers: Statistical physics, DFT, COSMO-RS, and AIM studies. <b>2022</b> , 364, 119956	O
329	Bromochlorodifluoromethane interaction with pristine and doped BN nanosheets: A DFT study. <b>2022</b> , 10, 108367	1
328	Peripheral group engineering on hole-transporting materials in perovskite solar cells: Theoretical design and experimental research. <b>2022</b> , 206, 110604	2
327	Nonlinear optical and quantum chemical studies of Palladium benzimidazole Schiff base complex. <b>2022</b> , 151, 107012	1

326	Cytotoxic effects of Pd(II) complexes on cancer and normal cells: Their DNA & amp; BSA adduct formation and theoretical approaches. <b>2022</b> , 128, 106093	1
325	Incorporating hard-soft acid-base theory in multi-aspect analysis of the adsorption mechanism of aqueous heavy metals by graphene oxide. <b>2022</b> , 170, 110934	О
324	Regioselective synthesis of spirooxindole-pyrolidine via (GAP) chemistry process: Experimental and DFT study. <b>2022</b> , 1270, 133891	
323	Synthesized thiazole-based hydrazides and their spectral characterization along with biological studies: Promising quantum chemical insights. <b>2022</b> , 1270, 133923	3
322	Molecular dynamic simulations and computational DFT of adsorption performances of malachite green on the metal fluorides in aqueous medium. <b>2022</b> , 1270, 133924	0
321	Observation of new mesophases and detailed QM analysis of terephthalylidene-bis-[4-n-decylaniline] liquid crystal molecule. <b>2022</b> , 1269, 133815	
320	Density Functional Theory Study of the Regioselectivity in Copolymerization of bis-Styrenic Molecules with Propylene Using Zirconocene Catalyst. <b>2022</b> , 12, 1039	1
319	Insights into solvent effects on molecular properties, physicochemical parameters, and NLO behavior of brinzolamide, a bioactive sulfonamide: A computational study. <b>2022</b> , 99, 100738	О
318	Theoretical insight and molecular recognition of oxatub[4]arene-based organic macrocycle as a supramolecular host for antipsychotic drug risperidone. <b>2022</b> , 366, 120195	О
317	An experimental and theoretical investigation of cationic azine dye adsorption on natural sepiolite in single and multi-component systems. <b>2022</b> , 187, 507-515	1
316	Structure, electronic and optical properties of chalcopyrite-type semiconducting materials XGaY2 (X $'$ = $'$ Cu, Ag, Au; Y $'$ = $'$ S, Se, Te) for solar cell applications: A DFT study. <b>2022</b> , 646, 414305	O
315	Photochemical reactions of dinuclear organometallic complexes with diphenyl dichalcogenides. <b>2022</b> , 982, 122517	О
314	Investigation of the substituted Litanium nanocages using computational chemistry. 2023, 118, 108317	O
313	Nitrobenzamido substitution on thiophene-3-carboxylate: Electrochemical investigation, antioxidant activity, molecular docking, DFT calculations. <b>2023</b> , 1271, 134030	О
312	Green synthesis of chromonyl chalcone and pyrazoline as potential antimicrobial agents IDFT, molecular docking and antimicrobial studies. <b>2023</b> , 1271, 133993	1
311	Efficient one-pot synthesis, characterization and IDFT study of solvents polarity effects on the structural, energetic and thermodynamic proprieties of (a-methylamino-ethyl)-phosphonic acid dimethyl ester. <b>2023</b> , 1272, 134165	О
310	Synthesis of new sulfamate linked 4-hydroxycoumarin conjugates as potent anti-∃-amylase agents: In vitro approach coupled with molecular docking, DFT calculation and chemoinformatics prediction. <b>2023</b> , 1271, 134020	o
309	Unveiling the non-polar [3+2] cycloaddition reactions of cyclic nitrones with strained alkylidene cyclopropanes within a molecular electron density theory study. <b>2022</b> , 12, 25354-25363	О

308	Quantum dot decorated polyaniline plastic as a multifunctional nanocomposite: experimental and theoretical approach. <b>2022</b> , 12, 24063-24076	1
307	Computational study of quinoline-based thiadiazole compounds as potential antileishmanial inhibitors. <b>2022</b> , 46, 17554-17576	O
306	Unveiling the [3+2] cycloaddition between difluoromethyl diazomethane and 3-ylideneoxindole from the perspective of molecular electron density theory.	2
305	Ni(i)IIPA stabilization by hydrogen bond formation on the second coordination sphere: a DFT characterization. <b>2022</b> , 51, 12585-12595	O
304	New venues in electron density analysis. 2022, 24, 21538-21548	1
303	Electronic properties of amino acids and nucleobases: similarity classes and pairing principles from chemical reactivity indices. <b>2022</b> , 24, 22477-22486	2
302	Impact of Doping on the Optoelectronic, Electronic and Nonlinear Optical Properties and on the Reactivity of Photochromic Polymers Containing Styrylquinoline Fragments.	0
301	DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science.	9
300	Coronene-based quantum dots for the delivery of the doxorubicin anticancer drug: a computational study. <b>2022</b> , 46, 18518-18534	0
299	Theoretical investigations on the antioxidant potential of 2,4,5-trihydroxybutyrophenone in different solvents: A DFT approach. <b>2022</b> , 4, 100515	1
298	Spectroscopic and quantum chemical investigations to explore the effect of intermolecular interactions in a diuretic drug: Hydrochlorothiazide. <b>2023</b> , 285, 121931	0
297	Experimental and Quantum Chemical Approaches for Hydrazide-based Crystalline Organic Chromophores: Synthesis, SC-XRD, Spectroscopic and Nonlinear Optical Properties. <b>2023</b> , 1272, 134208	O
296	A computational finding on the effect of Econjugated acceptors in thiophene-linked coumarin dyes for potential suitability in DSSC application. <b>2023</b> , 435, 114300	0
295	Theoretical Analysis of the Adsorption of Pentachlorophenol and 6-OH-BDE-47 (6-Hydroxy-2,2[4,4ETetrabromodiphenyl Ether) by Boron Nitride Nanotubes Decorated with Double-Decker Lanthanide(III) Phthalocyanine Complexes. <b>2022</b> , 12, 1205	О
294	A B3LYP/DFT Study on the Structure Activity Relationship for Benzimidazole Derivatives in Water Solution. <b>2022</b> , 16, 579-589	0
293	Zinc oxide nanoclusters and their potential application as CH 4 and CO 2 gas sensors: Insight from DFT and TD-DFT. <b>2022</b> , 43, 1839-1847	O
292	A DFT approach to the adsorption of the Levodopa anti-neurodegenerative drug on pristine and Al-doped boron nitride nanotubes as a drug delivery vehicle.	О
291	Charge transfer at finite temperature: the " ��big is good" principle.	1

290	Unveiling the Origin of the Selectivity and the Molecular Mechanism in the [3+2] Cycloaddition Reaction of N-aryl-C-carbamoylnitrone with N-arylitaconimide. <b>2022</b> , 3, 281-292	0
289	Self-assembly of new cobalt complexes based on [Co (SCN)4], synthesis, empirical, antioxidant activity, and quantum theory investigations. <b>2022</b> , 12,	1
288	Effects of boron/nitrogen/phosphorus doping on the scavenging action of armchair single-walled carbon nanotubes (armchair-SWCNT) for OH radicals: a DFT study.	0
287	Species resolved interaction mechanism between graphene oxide and Cu(II) in aqueous solution with implications on wastewater remediation.	О
286	Electrophilicity of Hoveyda-Grubbs Olefin Metathesis Catalysts as the Driving Force that Controls Initiation Rates.	0
285	Application of catalysts in the synthesis of 4-(4-(dimethylamino)benzylidene)-3-methylisoxazol-5(4H)-one: experimental and theoretical studies. <b>2022</b> , 128,	o
284	Solvent Effects in the Regioselective N-Functionalization of Tautomerizable Heterocycles Catalyzed by Methyl Trifluoromethanesulfonate: A Density Functional Theory Study with Implicit Solvent Model. <b>2022</b> , 10, 172	0
283	Coupling of pseudoradical centers in the synthesis of oxazine fused-spiroindoline: a two-stage one-step double cyclization. <b>2022</b> , 134,	О
282	In Silico Screening of Active Compounds in Garri for the Inhibition of Key Enzymes Linked to Diabetes Mellitus.	1
281	Inorganic resins enable the increased purification efficiency of 82Sr from rubidium targets for use in PET imaging isotope production.	О
280	Biological Activity of Some Thiazolyl-thiadiazines as BACE-1 Inhibitors for Alzheimer Disease in the Light of DFT based Quantum Descriptors.	O
279	Reversible hydrogen storage capacity of vanadium decorated small boron clusters (BnV2, n=6-10): A dispersion corrected density functional study. <b>2022</b> , 113899	О
278	Self-Assembly of Matchstick-Shaped Inorganic Nano-Surfactants with Controlled Surface Amphiphilicity.	0
277	From Density Functional Theory to Conceptual Density Functional Theory and Biosystems. <b>2022</b> , 15, 1112	О
276	On the Periodicity of the Information Theory and Conceptual DFT-Based Reactivity Descriptors. <b>2022</b> , 126, 6801-6813	О
275	Theoretical Investigation on the Selective Hydroxyl Radical <b>I</b> hduced Decolorization of Methylene-Blue-Dyed Polymer Films. <b>2022</b> , 10, 169	o
274	Synthesis, spectroscopic characterization, density functional theory study, antimicrobial and antioxidant activities of curcumin and alanine-curcumin Schiff base. 1-16	1
273	HYDROGEN ADSORPTION AND STORAGE ON PALLADIUM-FUNCTIONALIZED C20 BOWL AND C20H10 BOWL MOLECULE INCLUDING HYDROGEN SATURATION. <b>2022</b> , 63, 1399-1408	О

272	H2 and CO adsorption ability of cationic lithiated carbenes: A computational study. 2022,	О
271	A DFT study on adsorption of diazinon and fenitrothion on nanocages B12N12 and B12P12.	O
270	Unravelling the Effect of Donor-EAcceptor Architecture in Designing 1,3-Indanedione Based Sensitizers for DSSC Applications. <b>2022</b> , 114328	0
269	Electrochemistry, DFT Calculations, and Antioxidant Capability of Cobalt Cefazolin Complex. 1083-1090	O
268	Seed-Mediated Synthesis of Photoluminescent CuZn[hB Nanoplatelets.	О
267	DFT-based computations on some structurally related N-substituted piperazines. 2022, 100766	1
266	Exploring the Fe doped borazine system as a promising CFC adsorbent: A DFT study. <b>2022</b> , 1217, 113903	0
265	Interatomic potentials: achievements and challenges. 2023, 8,	О
264	New organic dye-sensitized solar cells based on the DAA structure for efficient DSSCs: DFT/TD-DFT investigations. <b>2022</b> , 12, 30626-30638	0
263	Organo-metallic electrolyte additive for regulating hydrogen evolution and self-discharge in MgBir aqueous battery. <b>2022</b> , 46, 19950-19962	О
262	Conceptual Density Functional Theory. 2022,	0
261	Chemical Bonding With Plane Waves. <b>2022</b> ,	O
260	Synthesis and structural characteristic of pyridine carboxylic acid adducts with squaric acid.	О
259	A theoretical study on aza-Michael additions. <b>2022</b> , 141,	1
258	Silylium ion migration dominated hydroamidation of siloxy-alkynes. <b>2022</b> , 5,	0
257	AlCl3-Catalyzed Cascade Reactions of 1,2,3-Trimethoxybenzene and Adipoyl Chloride: Spectroscopic Investigations and Density Functional Theory Studies. <b>2022</b> , 7, 38882-38893	O
256	[3 + 2] Cycloadditions in Asymmetric Synthesis of Spirooxindole Hybrids Linked to Triazole and Ferrocene Units: X-ray Crystal Structure and MEDT Study of the Reaction Mechanism. <b>2022</b> , 14, 2071	0
255	Theoretical calculations of formation and reactivity of o -quinomethide derivatives of resorcin[4]arene with reference to empirical data. <b>2022</b> , 9,	1

254	Anti-proliferative action, molecular investigation and computational studies of novel fused heterocyclic cellulosic compounds on human cancer cells. <b>2022</b> ,	О
253	Superstrong Chemical Bonding of Noble Gases with Oxidoboron (BO+) and Sulfidoboron (BS+). <b>2022</b> , 126, 7888-7900	О
252	Thermodynamics of the Metal Carbonates and Bicarbonates of Mn, Co, Ni, Cu, and Zn Relevant to Mineral Energetics. <b>2022</b> , 126, 7874-7887	1
251	Application of Fundamental Chemical Principles for Solvation Effects: A Unified Perspective for Interaction Patterns in Solution. <b>2022</b> , 126, 8864-8872	1
250	Ranking the energy minima of the 20 natural amino acids using conceptual tools. <b>2022</b> , 141,	0
249	Understanding the origin of reactivity, mechanism and regioselectivity of the [3+2] cycloaddition reaction between nitrile imine and pyrrolopyrazine.	O
248	A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of an Azomethine Ylide with an Electrophilic Ethylene Linked to Triazole and Ferrocene Units. <b>2022</b> , 27, 6532	1
247	Anti-Inflammatory Nanocarriers Based on SWCNTs and Bioactive Molecules of Oregano: An In Silico Study. <b>2022</b> , 2, 176-185	О
246	Oxidation state-specific fluorescent copper sensors reveal oncogene-driven redox changes that regulate labile copper(II) pools. <b>2022</b> , 119,	1
245	Synthesis, Anticancer, Antioxidant, Anti-Inflammatory, Antimicrobial Activities, Molecular Docking, and DFT Studies of Sultams Derived from Saccharin. <b>2022</b> , 27, 7104	О
244	Two-Site OH Addition to an Iridium Complex Featuring a Nonspectator Tricoordinate Phosphorus Ligand.	1
243	Decomposition of formic acid via carboxyl mechanism on the graphene nanosheet decorated by Cr, Mn, Fe, Co, Ni, Pd, Ag, and Cd metals: A DFT study. <b>2022</b> ,	O
242	Carica papaya Seeds and Its Active Constituent Benzyl Isothiocyanate against Corrosion of Aluminum. <b>2022</b> , 58, 491-508	О
241	Synergism of 2-mercaptobenzimidazole and oleic imidazoline on corrosion inhibition of carbon steel in CO2 -saturated brine solutions. <b>2022</b> , 120645	O
240	Insight into designing of 2-pyridone derivatives for COVID-19 drug discovery - A computational study.	О
239	Brief Research on the Biophysical Study and Anticancer Behavior of Pt(II) Complexes: Their DNA/BSA Binding, Molecular Docking, and Cytotoxic Property.	O
238	Small molecule sensors for the colorimetric detection of Copper(II): A review of the literature from 2010 to 2022. <b>2022</b> , 110881	O
237	CHEMISORPTION OF C2H2 ON C20 BOWL: A COMPUTATIONAL INVESTIGATION. <b>2022</b> , 63, 1600-1609	O

236	New Theoretical Insights about Anticorrosive Effects and Adsorption Mechanism of Some ⊞-Amino Acids on Al Surface: DFT, MEP, FMO, NBO, QSAR, Fukui Functions and Monte Carlo Simulation.	O
235	Protein-Ligand Based Pharmacophore Approach against ERK5 Involved in Breast Cancer; In-Silico Study of Flavonoids from Blighia sapida.	O
234	Cheminformatics Study on Structural and Bactericidal Activity of Latest Generation	0
233	Electronegativity provides the relationship between formal charge, oxidation state, and actual charge.	O
232	In silico designing of Si- and Ge-doped imidazolium: a new heterocyclic aromatic superacid. <b>2022</b> , 141,	O
231	Identifying Potential p53-MDM2 Interaction Antagonists: An Integrated Approach of Pharmacophore-Based Virtual Screening, Interaction Fingerprinting, MD´ Simulation and DFT Studies. <b>2022</b> , 7,	O
230	Electronic Spectra (Experimental and Simulated), and DFT Investigation of NLO, FMO, NBO, and MESP Characteristics of Some Biphenylcarboxaldehydes. 1-14	О
229	A first principle study to investigate structural, electronic and optical properties of pristine and valency comparable Co, P decorated graphene like boron nitride (BN) nanosheets. 1-14	O
228	Novel endohedrally and exohedrally metals (Li, Na, and K, Ag) doped (15-crown-5) with remarkable electronic, static and dynamic NLO response. <b>2022</b> , 170169	O
227	Modeling of pristine, Ir- and Au-decorated C60 fullerenes as sensors for detection of hydroxyurea and nitrosourea drugs. <b>2022</b> , 10, 108802	4
226	A novel spirooxazine derivative as a colorimetric probe for Fe2+ and Pb2+ determination on microfluidic paper-based analytical device (PAD) for maintaining in photochromic efficiency. <b>2022</b> , 208, 110869	0
225	Graphene oxide-safranin modified@polyacrylonitrile membranes for water purification: Reuse and mechanism based on theoretical calculations and XPS analysis. <b>2022</b> , 50, 103248	1
224	Pd nanoparticle-mediated acetone sensing performance improvement of SnO2 substrate: A combined DFT and experimental study. <b>2022</b> , 44, 131-143	O
223	Diaminoalkanes functionalized graphene oxide as corrosion inhibitors against carbon steel corrosion in simulated oil/gas well acidizing environment. <b>2023</b> , 630, 591-610	1
222	Feasible synthesis of bifunctional polysilsesquioxane microspheres for robust adsorption of Hg(II) and Ag(I): Behavior and mechanism. <b>2023</b> , 442, 130121	1
221	A density functional theory study of H3+ and Li3+ clusters: Similar structures with different bonding, aromaticity, and reactivity properties. <b>2023</b> , 237-245	O
220	Polarizability of atoms and atomic clusters. <b>2023</b> , 313-320	O
219	Conceptual density functional theory and all metal aromaticity. 2023, 87-98	O

218	Zintl cluster as a building block of superalkali, superhalogen, and superatom. 2023, 333-344	О
217	Investigation of embelin synthetic hybrids as potential COVID-19 and COX inhibitors: Synthesis, spectral analysis, DFT calculations and molecular docking studies. <b>2023</b> , 1273, 134356	2
216	Hydrogen trapping potential of a few novel molecular clusters and ions. 2023, 297-312	O
215	Synthesis, nonlinear optical analysis and DFT studies of D <b>D</b> and A <b>A</b> configured Schiff bases derived from bis-phenylenediamine. <b>2022</b> , 12, 32185-32196	О
214	Combination of Explainable Machine Learning and Conceptual Density Functional Theory: Applications for the Study of Key Solvation Mechanisms.	О
213	Exploration of electronic and non-linear optical properties of novel 4-Aryl-2-methylpyridine based compounds synthesized via high-yielding Pd(0) catalysed reaction. <b>2023</b> , 1274, 134469	O
212	Quantum Chemical Benchmark Study on Valdecoxib, a Potent and Selective Inhibitor of COX-2, and its Hydroxylated Derivative. <b>2022</b> , 43, 221-231	0
211	A Molecular Electron Density Theory Study of the Polar Diels-Alder Reaction of Naphtoquinone:Cr(CO)3 Complex with Cyclic Dienes. 1-17	O
210	Unveiling the zwitterionic and stepwise mechanism for the domino reactions of amidine with 1,2,4,5- and 1,2,3,5-tetrazines.	0
209	Quantum Chemical Investigation of the New 1,2,4-Triazoles and Their Derivatives: Solvent and Substituent Effects. <b>2022</b> , 96, 2441-2450	O
208	Molecular and periodic DFT calculations of the corrosion protection of Fe(110) by individual components of Aerva lanata flower as a green corrosion inhibitor. <b>2022</b> , 101566	1
207	On the possibility of using the Ti@Si16 superatom as a novel drug delivery carrier for different drugs: A DFT study. <b>2022</b> , 108378	O
206	Efficient adsorption of antibiotics and heavy metals from aqueous solution by structural designed PSSMA-functionalized-chitosan magnetic composite. <b>2022</b> , 140417	1
205	Biobased additives for asphalt applications produced from the hydrothermal liquefaction of sewage sludge. <b>2022</b> , 108974	O
204	Studying the Temperature Influence on Carbon Steel in Sour Petroleum Media Using Facilely-Designed Schiff Base Polymers as Corrosion Inhibitors. <b>2022</b> , 134518	3
203	An account of noncovalent interactions in homoleptic palladium(II) and platinum(II) complexes within the DFT framework: A correlation between geometries, energy components of symmetry-adapted perturbation theory and NCI descriptors. <b>2022</b> , 8, e11408	O
202	Structural, electronic, spectroscopic and molecular docking analysis of novel hetero oxetane ring compound. <b>2022</b> , 1217, 113919	1
201	Impact of doping on the optoelectronic, electronic and nonlinear optical properties and on the reactivity of photochromic polymers containing styrylquinoline fragments: Hartree-Fock and DFT study. <b>2022</b> , 8, e11491	1

200	Conceptual Density Functional Theory for Temporary Anions Stabilized by Scaled Nuclear Charges.	0
199	Theoretical Study of Cyano-Promoted Intramolecular Aza-DielsAlder Reaction.	O
198	In-silico and in-detail experimental interaction studies of new antitumor Zn(II) complex with CT-DNA and serum albumin. 1-18	О
197	Quantum chemical study on the structural mechanism, III interactions and hydrogen bonding network of 2, 6-diamine-7H-purine molecule: using molecular modeling.	О
196	The Consequences of Water Interactions with Nitrogen-Containing Carbonaceous Quantum Dots The Mechanistic Studies. <b>2022</b> , 23, 14292	1
195	What is the role of phytochemical compounds as capping agents for the inhibition of aggregation in the green synthesis of metal oxide nanoparticles? A DFT molecular level response. <b>2022</b> , 110243	O
194	Manipulation of N-heterocyclic carbene reactivity with practical oriented electric fields. <b>2022</b> , 25, 375-383	O
193	Impacts of External Fields on Aromaticity and Acidity for Benzoic Acid: A Density Functional Theory, Conceptual Density Functional Theory and Information-Theoretic Approach Study.	O
192	Biophysical investigation of the interaction between NSAID ibuprofen and cationic biodegradable Cm-E2O2-Cm gemini surfactants. <b>2023</b> , 370, 120972	1
191	Adsorption and electronic properties of pristine and Al-doped C60 fullerenes using N2O molecule: A theoretical study. <b>2023</b> , 369, 120855	O
190	Theoretical investigation of intermolecular interactions between CNT, SiCNT and SiCGeNT nanomaterials with vinyl chloride molecule: A DFT, NBO, NCI, and QTAIM study. <b>2023</b> , 131, 109602	O
189	Unveiling the high reactivity of experimental pseudodiradical azomethine ylides within molecular electron density theory. <b>2022</b> , 25, 314-325	1
188	Magnetic graphene oxide-chitosan nanohybrid for efficient removal of aqueous Hg(I) and the interaction mechanism. <b>2023</b> , 370, 121050	О
187	Synthesis, spectroscopic, SC-XRD/DFT and non-linear optical (NLO) properties of chromene derivatives. <b>2022</b> , 13, 464-477	О
186	Density functional theory study of the sensing of ozone gas molecules by using fullerene-like Group-III nitride nanostructures. <b>2023</b> , 650, 414553	О
185	Substituted naphthoxy-phthalonitrile derivatives: Synthesis, substituent effects, DFT, TD-DFT Calculations, antimicrobial properties and DNA interaction studies. <b>2023</b> , 102, 107798	O
184	Crystal growth, Hirshfeld surface, quantum chemical calculations, optical, photoluminescence and thermal analyses of sodium D-isoascorbate monohydrate single crystal. <b>2023</b> , 1275, 134637	О
183	Molecular simulation investigations on interaction properties of the teriflunomidelhitosan complex in aqueous solution. <b>2023</b> , 174, 111171	1

182	Selective adsorption of Pd(II) over Ag(I) in nitric acid solutions using nitrogen-donor-type adsorbents. <b>2023</b> , 308, 122943	1
181	A comparative structural analysis of arylsulfonamide chalcones with potential as a biofuel additive. <b>2023</b> , 1276, 134736	Ο
180	Studies on the DFT calculations and molecular docking of versatile molecular sensor 1-(6-Aminopyridin-2-yl) -3-(4-nitrophenyl) urea. <b>2023</b> , 6, 100139	0
179	Advances in reaction-based synthetic fluorescent probes for studying the role of zinc and copper ions in living systems. <b>2022</b> ,	Ο
178	A theoretical and practical inclusive study of the effect of some factors on the ionization constants of some aromatic imines by potentiometric titration. <b>2022</b> ,	0
177	Experimental and Theoretical Studies of Inhibitive Behaviour of Millet Starch on the Corrosion of Aluminium in Sulphuric Acid Environment. 8, 1-13	Ο
176	Preparation and properties of phosphinic acidfunctionalized polyacrylonitrile hollow fiber membrane for heavy metal adsorption.	0
175	Manganese Molybdate Cathodes with Dual-Redox Centers for Aqueous Zinc-Ion Batteries: Impact of Electrolyte on Electrochemistry. <b>2022</b> , 10, 16197-16213	O
174	Molecular charge distributions in strong magnetic fields: a conceptual and current DFT study.	О
173	A conceptual density functional theory approach to substituent effects in fluorescence processes: The case of naphthalimide derivatives.	O
172	Comprehensive Assessment of Biomolecular Interactions of Morpholine-Based Mixed Ligand Cu(II) and Zn(II) Complexes of 2,2?-Bipyridine as Potential Anticancer and SARS-CoV-2 Agents: A Synergistic Experimental and Structure-Based Virtual Screening. <b>2022</b> , 2022, 1-29	O
171	Chlorine counterion effect into the supramolecular arrangement of phenylephrine solid state. <b>2022</b> , 113992	O
170	A theoretical evaluation for new fused remote N-heterocyclic silylenes (RNHSis) using density functional theory.	О
169	Synthesis, characterization of some substituted Quinolines derivatives: DFT, Computational, in Silico ADME, Molecular Docking and Biological Activities. <b>2022</b> , 100977	O
168	Density Functional Theory Analysis of the Copolymerization of Cyclopropenone with Ethylene Using a Palladium Catalyst. <b>2022</b> , 14, 5273	1
167	Charge Transfer as Bridging Correlator for DSSC Efficiency and NLO Property. <b>2022</b> , 7,	O
166	Anti-proliferative activity, Molecular docking study of Novel synthesized Ethoxyphenylbenzenesulfonamide with Computational Calculations. <b>2022</b> , 134871	1
165	Ligands as Matchmakers[Alloying from a Physical Mixture of Metal Nanoparticle Dispersions by Digestive Ripening. <b>2022</b> , 38, 15917-15924	O

164	Pseudo-Protic Ionic Liquids for the Extraction of Metals Relevant for Urban Mining.	1
163	Dual Ligand Capped Quantum Dots Improving Loading Amount for High-Efficiency Quantum Dot-Sensitized Solar Cells. 647-656	О
162	Strychnos alkaloids: total synthesis, characterization, DFT investigations, and molecular docking with AChE, BuChE, and HSA. <b>2022</b> , 8, e11990	0
161	Unveiling novel reactivity of P/Al frustrated Lewis pair: ring size-dependent activation of cyclic ethers/thioethers and CO2 insertion therein. <b>2022</b> , 134,	О
160	In pursuit of novel pyriporphyrin porphyrin ring expansion congener containing a built-in pyridine moiety by CH radical: a DFT investigation.	Ο
159	The effect of alkali metals, carbocations, and metallocenes substitutes on two Etarrabiose disaccharide derivatives: a density functional study.	O
158	Copper(II) chelates derived from an N,N,O-tridentate 2-pyridinecarboxaldehyde-N4-phenylsemicarbazone: Synthesis, spectral aspects, crystal structure, FMO and NBO analysis. <b>2022</b> , 134866	0
157	How a Chromium Tricarbonyl Complex Catalyzes the [3 + 2] Cycloaddition Reaction of N-Substituted Phenylnitrones with Styrene: A Molecular Electron Density Theory Analysis. <b>2022</b> , 41, 3809-382	2 <sup>O</sup>
156	Probing Diversity in Binding Affinities of Polymorphs of an Anticancer Agent against Human 眶nolase: A Quantum Crystallographic Perspective.	0
155	Substituent effect on the photoinduced geometrical changes of Cu(I)Phen2 complexes. 2022, 111806	О
154	Identification of potential inhibitors of omicron variant of SARS-Cov-2 RBD based virtual screening, MD simulation, and DFT. 10,	О
153	Structure and Electronic Properties of Metalloboranes with General Formula Cp* 3 (EH)M 3 B 8 H 8 (M=Cr, Mo and W): The Effect of the Size of the Metal. <b>2022</b> , 7,	О
152	Delocalization state-induced selective bond breaking for efficient methanol electrosynthesis from CO2.	2
151	A Selective and <b>D</b> ff <b>D</b> n <b>I</b> Fluorescent Chemosensor Based on Fluorescein for Al3+: Synthesis, Characterization, Spectroscopy Analyses, and DFT Calculation.	O
150	Atoms-In-Molecules[Faces of Chemical Hardness by Conceptual Density Functional Theory. <b>2022</b> , 27, 8825	0
149	Absolute Hydration Free Energy of Small Anions and the Aqueous pKa of Simple Acids. <b>2022</b> , 126, 9190-9206	0
148	Synthesis and Crystal Structure of Adamantylated 4,5,6,7-tetrahalogeno-1H-benzimidazoles Novel Multi-Target Ligands (Potential CK2, M2 and SARS-CoV-2 Inhibitors). X-ray/DFT/QTAIM/Hirshfeld Surfaces/Molecular Docking Study. <b>2023</b> , 28, 147	1
147	Quantum chemical study of effect on adsorption properties of antituberculosis drug N-Cyclopentylidenepyridine-4-carbohydrazide interaction with CNT(C56H16). <b>2022</b> , 100851	O

146	Pyridine derivatives complexes of Co (II) and Ni (II) 3-Bromobenzoates: Crystal Structure, in silico Anti-SARS-CoV-2 potential, Serum Albumin Binding Properties and Cytotoxicity.	О
145	Degradation by hydrolysis of three triphenylmethane dyes: DFT and TD-DFT study. 2023, 142,	O
144	Spectroscopic, structural, and intermolecular interactions of 4-(2-hydroxy-3-methoxybenzylideneamino)-N-(5-methylisoxazol-3-yl)benzenesulfonamide enol-imine and keto-amine isomers. <b>2023</b> , 134978	О
143	Synthesis, X-Ray, Spectroscopic Characterization, Hirshfeld Surface Analysis, Molecular Docking, and DFT Calculations of a New Series of 3-Hydrazono and 3-Phenylhydrazono Isatin Derivatives. 1-18	О
142	Synthesis and Lewis Acidity of Fluorinated Triaryl Borates.	0
141	Spectroscopic and computational characterizations, Hirshfeld surface investigations, anticancer studies and molecular docking analysis of novel NLO 3-hydroxy-3?,4?,5,7-tetramethoxyflavone. <b>2023</b> , 46,	O
140	DFT study on molecular structure, spectroscopic properties, Hirshfeld surface and molecular docking reveals the potential of flavones based on experimental and theoretical investigations.	0
139	Unveiling the Mg(ii) promoted [3+2] cycloaddition reaction of mesitonitrile oxide to BaylisHilman adduct from the molecular electron density theory perspective.	o
138	Enhanced hydrogen storage performance of Li and Co functionalized h-GaN nanosheets: DFT study. <b>2023</b> , 108415	О
137	Structural, electronic and nonlinear optical properties, reactivity and solubility of the drug dihydroartemisinin functionalized on the carbon nanotube. <b>2023</b> , 9, e12663	1
136	Exploration on Ononin and Corylin molecule Against Anti-Influenza H1N1 A Virus via Molecular Docking, Molecular dynamics simulation and Binding free energy calculations.	O
135	Role of donors in triggering second order non-linear optical properties of non-fullerene FCO-2FR1 based derivatives: A theoretical perspective. <b>2023</b> , e13033	1
134	A biophysical approach of cytarabine anticancer drug insights into human serum albumin and checkpoint kinase 1. <b>2023</b> , 5, 100755	0
133	Synthesis, structural analysis, DFT study, antioxidant activity of metal complexes of N-substituted thiourea. <b>2023</b> , 231, 116274	O
132	Optical, electrochemical, and test strip methods for sensitive and selective detection of Cyanide ion using a multifunctional Eextended azaacene-based system. <b>2023</b> , 379, 133280	0
131	On the protonated forms of alkyl-bonded polycyclic aromatic heterocycles: Structure prediction and characterization using density functional theory. <b>2023</b> , 175, 111181	O
130	A Theoretical Study of Structure and Electronic Properties of Poly (e-Caprolactone) By Density Functional Study.	О
129	Corrosion inhibition mechanism of imidazole ionic liquids with high temperature in 20% HCl solution. <b>2023</b> , 29,	1

128	Accurate Metallmidazole Interactions.	0
127	Computational investigation of dimethoate and $\mathbb{C}$ y clodextrin inclusion complex: molecular structures, intermolecular interactions and electronic analysis.	О
126	Molecular Structure of 2-hydroxy-5-methyl-2-nitroazobenzene Isomer: DFT Insight.	O
125	Molecular modelling framework of metal-organic clusters for conserving surfaces: Langmuir sorption through the TD-DFT/ONIOM approach. 1-12	2
124	References. <b>2023</b> , 313-323	0
123	Properties of recombinant extracellular N-Terminal Domain of human high affinity copper transporter 1 (hNdCTR1) and its interactions with Cu(II) and Ag(I) lons.	o
122	New kind of electride sandwich complexes based on the cyclooctatetraene ligand M12(IB-C8H8)2M22 (M1 = Na, K and M2 = Ca, Mg): a theoretical study. <b>2023</b> , 25, 4710-4723	0
121	First Principal Study of Interaction of Copper Doped Gold Nanoclusters with Glycine. <b>2023</b> , 110435	O
120	Molecular engineering on D-EA organic dyes with flavone-based different acceptors for highly efficient dye-sensitized solar cells using experimental and computational study. <b>2023</b> , 29,	1
119	Spectroscopic, crystal structure and DFT-assisted studies of some nickel(II) chelates of a heterocyclic-based NNO donor aroylhydrazone: in vitro DNA binding and docking studies.	O
118	Computational Evaluation of Azadirachta indica-Derived Bioactive Compounds as Potential Inhibitors of NLRP3 in the Treatment of Alzheimer Disease. <b>2023</b> , 1-19	0
117	Understanding the mechanism and regio- and stereo selectivity of [3 + 2] cycloaddition reactions between substituted azomethine ylide and 3,3,3- trifluoro -1-nitroprop-1-ene, within the molecular electron density theory.	O
116	Effect of different end-capped donor moieties on non-fullerenes based non-covalently fused-ring derivatives for achieving high-performance NLO properties. <b>2023</b> , 13,	0
115	Organic Corrosion Inhibitors.	O
114	Unveiling the Electrophilic Aromatic Substitution Reactions of Pyridine Derivatives with Nitronium Ion through Molecular Electron Density Theory.	0
113	Development of quantitative structureEctivity relationship models based on electrophilicity index: a conceptual DFT-based descriptor. <b>2023</b> , 219-229	O
112	In-situ construction of grass-like hybrid architecture responsible for extraordinary corrosion performance: experimental and theoretical approach.	0
111	On the study of dye sensitized solar cells with high light harvesting efficiency and correlation of its chemical reactivity parameters with overall performance.	0

110	White light emission from coumarin and rhodamine derivatives based on RGB multicomponent system. <b>2023</b> , 439, 114577	О
109	Formation mechanism of a ternary nanohybrid based on magnetite-chitosan-graphene oxide according to HSAB theory. <b>2023</b> , 176, 111260	Ο
108	Synthesis, single crystal X-ray analysis and vibrational spectral studies of 3,4-di(1H-indol-3-yl)-1H-pyrrole-2,5-dione. <b>2023</b> , 1281, 135103	Ο
107	Self-assembly, physico-chemical characterization, biological, virtual screening, and computational approach of novel 2-amino pyridine derivatives. <b>2023</b> , 1281, 135049	O
106	Synthesis and structural characterization of a novel palbociclib-kaempferol cocrystal with improved tabletability and synergistic antitumor activity. <b>2023</b> , 1281, 135101	O
105	Density functional theory (DFT) computation of pristine and metal-doped MC59 (M = Au, Hf, Hg, Ir) fullerenes as nitrosourea drug delivery systems. <b>2023</b> , 158, 107362	1
104	Novel thiourea derivative compounds: Thermal behavior, biological evaluation, Hirshfeld surfaces and frontier orbitals analyses, in silico ADMET profiling and molecular docking studies. <b>2023</b> , 1280, 135086	О
103	Electronic Properties of Graphene Nanoribbons Doped with Pyrrole-Like Nitrogen. <b>2022</b> , 56, 406-410	O
102	Bond-bending isomerism and metallophilicity in metallialogen anions (Cu,Ag,Au)2X3 $\Pi$ X = F, Cl, Br, I, At. <b>2023</b> , 13, 7129-7134	0
101	A quinoline-benzotriazole derivative: Synthesis, crystal structure and characterization by using spectroscopic, DFT and molecular docking methods. <b>2023</b> , 5, 100916	O
100	Theoretical Insights into the Substitution Effect of Phenanthroline Derivatives on Am(III)/Eu(III) Separation. <b>2023</b> , 62, 2705-2714	0
99	Feather-weight cryostructured thiourea-chitosan aerogels for highly efficient removal of heavy metal ions and bacterial pathogens. <b>2023</b> , 235, 123910	1
98	Sm and S Co-doping to Construct Homo-hetero Cu Catalysts for Synergistic Enhancing CO 2 Electroreduction $\square$	0
97	Spectroscopic investigations, hirshfeld surface analysis, anticancer and molecular docking studies of new novel NLO 3-hydroxy-3?,4?,5,7-tetramethoxyflavone. <b>2023</b> , 101000	O
96	Synthesis of 3-amino-1,2,4-triazole-5-thiol functionalized p-phenylenediamine covalent organic polymer as a highly selective adsorbent for Hg2+ ions. <b>2023</b> , 186, 105575	0
95	Sorption and desorption performance of La3+/Bi3+ by surface-modified activated carbon for potential application in medical 225Ac/213Bi generators. <b>2023</b> , 464, 142456	O
94	Self-assembled quantum dots decorated polypyrrole based multifunctional nanocomposite. <b>2023</b> , 666, 131241	О
93	Optimized Baccharis dracunculifolia extract as photoprotective and antioxidant: In vitro and in silico assessment. <b>2023</b> , 440, 114654	Ο

92	Effect of silver nanoparticle size on interaction with artemisinin: First principle study. 2023, 11, 100104	О
91	Physicochemical properties, drug likeness, ADMET, DFT studies, and in vitro antioxidant activity of oxindole derivatives. <b>2023</b> , 104, 107861	O
90	Crystal structure, spectroscopic analysis, electronic properties and molecular docking study of costunolide for inhibitor capacity against Onchocerca volvulus main protease. <b>2023</b> , 1282, 135185	0
89	K2(H2O)WO3F2: A new nonlinear optical material with remarkable second-harmonic generation response and enhanced laser damage threshold. <b>2023</b> , 945, 169288	O
88	Corrosion protection studies of different alloys in 1´ M HCl by benzimidazole derivative: Combined molecular dynamic simulations/DFT. <b>2023</b> , 11, 109642	0
87	Quantum chemical, spectroscopic and molecular docking studies on methyl 2-chloro-6-methyl pyridine-4-carboxylate: A potential inhibitor for irritable bowel syndrome. <b>2023</b> , 294, 122544	O
86	Chemical background of silver nanoparticles interfering with mammalian copper metabolism. <b>2023</b> , 451, 131093	1
85	Thiazole-pyrazoline hybrids as potential antimicrobial agent: Synthesis, biological evaluation, molecular docking, DFT studies and POM analysis. <b>2023</b> , 1282, 135191	O
84	Design, synthesis, and computational studies of novel imidazo[1,2-a]pyrimidine derivatives as potential dual inhibitors of hACE2 and spike protein for blocking SARS-CoV-2 cell entry. <b>2023</b> , 1285, 135525	О
83	Density functional modeling of the binding energies between aluminosilicate oligomers and different metal cations. 10,	O
82	Molecular modeling and solubility of olopatadine hydrochloride polymorphs. 2023, 1224, 114110	O
81	Iron-ligand complex, an efficient inhibitor of steel corrosion in hydrochloric acid media. <b>2023</b> , 1284, 135434	O
80	Synthesis, biological activities, molecular docking, theoretical calculations of some 1,3,4-oxadiazoles, 1,2,4-triazoles, and 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazines derivatives. <b>2023</b> , 1283, 135238	О
79	Combination mechanism of the ternary composite based on Fe3O4-chitosan-graphene oxide prepared by solvothermal method. <b>2023</b> , 231, 123337	O
78	Reduction potential of benzophenones, hydroxyphenones and bis(2-hydroxyphenone)copper molecules. <b>2023</b> , 443, 141931	O
77	Phytochemical components of Allium Jesdianum flower as effective corrosion-resistant materials for Fe(1 1 0), Al(1 1 1), and Cu(1 1 1): DFT study. <b>2023</b> , 16, 104625	O
76	Efficient synthesis of chromeno[2,3-b]pyridine derivatives using Zn(OTf)2 as a catalyst: DFT computations, molecular docking and ADME studies. <b>2023</b> , 375, 121364	0
75	Optimization study of pharmaceuticals pollutants adsorption onto large surface area walnut shells activated carbon: Experimental design, Mechanism and DFT calculations.	O

74	(ZnO)42 nanocluster: a novel visibly active magic quantum dot under first principle investigation. <b>2023</b> , 142,	O
73	3D/2D Core/Shell Perovskite Nanocrystals for High-Performance Solar Cells. 2207312	O
72	Quantum Chemical Analysis and Effect of Super Alkali/Super Halogen Doping on the Opto-Electronic Properties of L-Lysine p-Nitrophenolatemonohydrate (LLPNP) Using First Principle. 1-23	O
71	Experimental and Theoretical Study of Tetrel Bonding and Noncovalent Interactions in Hemidirected Lead(II) Phosphorodithioates: An Implication on Crystal Engineering. <b>2023</b> , 23, 2138-2154	O
70	In Silico Prediction, Characterization and Molecular Docking Studies on New Benzamide Derivatives. <b>2023</b> , 11, 479	O
69	New Insights into the Formation of CH3OCH3 and CH3SCH3 without and with the Assistance of Na+ Ions and Some Implications for Interstellar Chemistry: An In Silico Approach. <b>2023</b> , 7, 388-403	O
68	Fluorine-selective post-plasma chemical ionization for enhanced elemental detection of fluorochemicals. <b>2023</b> , 38, 854-864	O
67	Doping of Graphene Nanostructure with Iron, Nickel and Zinc as Selective Detector for the Toxic Gas Removal: A Density Functional Theory Study. <b>2023</b> , 9, 20	O
66	Design, Synthesis, and Optical and Electrochemical Properties of DA Type Organic Dyes with Carbazole-Based Donor Units for Efficient Dye-Sensitized Solar Cells: Experimental and Theoretical Studies. <b>2023</b> , 52, 2525-2543	O
65	Theoretical investigation for dye-sensitized solar cells: effect of donor variation on the optoelectronic properties and charge transfer parameters. <b>2023</b> , 49, 1731-1754	O
64	Vibrational Spectroscopies, Global Reactivity, Molecular Docking, Thermodynamic Properties and Linear and Nonlinear Optical Parameters of Monohydrate Arsenate Salt of 4-Aminopyridine.	O
63	A simple uric acid assay by using 3-hydroxytyramine as a chromogenic colorimetric sensor in human serum samples: Density functional theory supported mechanistic approach. <b>2023</b> , 70, 894-908	O
62	A comprehensive DFT study on organosilicon-derived fungicide flusilazole and its germanium analogue: A computational approach to Si/Ge bioisosterism. <b>2023</b> , 100, 100939	O
61	Photocatalytic degradation and pollutant-oriented structure-activity analysis of carbamazepine, ibuprofen and acetaminophen over faceted TiO2. <b>2023</b> , 11, 109553	O
60	Comparative Study of Molecular Docking, Structural, Electronic, and Fukui Function Studies on Favipiravir and its Newly Designed Derivatives (Potential Inhibitors) for COVID-19 Protease. <b>2023</b> , 407,	O
59	Reconsideration of chemical indices in conceptual density functional theory. <b>2023</b> , 142,	O
58	Time-Dependent Density Functional Theory, AIM Analysis, NLO, and Thermodynamic Properties of Propofol and Adsorption Effects of Propofol Drug over Carbon Nanotube (C56H16) as the Factor of Drug Delivery System. <b>2023</b> , 407,	О
57	DFT CALCULATIONS IN MONOMERIC AND DIMERIC FORMS OF N-BENZYLMALEIMIDE (NBM) COMBINED WITH VIBRATIONAL SPECTROSCOPIC PARAMETERS.	Ο

56	Exploring the Interaction Between the Newly Designed Antitumor Zn(II) Complex and CT-DNA/BSA: Spectroscopic Methods, DFT Computational Analysis, and Docking Simulation.	O
55	Co3O4 quantum dot decorated polypyrrole nanocomposites as a flexible, conducting, anticorrosive and antibacterial agent: sustainable experimental and theoretical approach.	O
54	Inhibition of corrosion of an aluminum alloy by Rosemary and Eucalyptus extracted oils in 1M hydrochloric acid medium: Experimental and theoretical study.	О
53	Theoretical descriptions of novel silicon analogs of cyclo[18]carbon.	O
52	Barrier Height Prediction by Machine Learning Correction of Semiempirical Calculations. <b>2023</b> , 127, 227	<b>1-2283</b> o
51	A dispersion-corrected DFT calculations on encapsulation of Favipiravir drug used as antiviral against COVID-19 into carbon-, boron-, and aluminum-nitride nanotubes for optimal drug delivery systems combined with molecular docking simulations.	O
50	Graphene Embedded with Transition Metals for Capturing Carbon Dioxide: Gas Detection Study Using QM Methods. <b>2023</b> , 5, 403-417	O
49	Quantitative Solvation Energies from Gas-Phase Calculations: First-Principles Charge Transfer and Perturbation Approaches. <b>2023</b> , 127, 2546-2551	O
48	DFT study of the conformation, hydrogen bonds, IR, Raman, and NMR spectra of 1,3-disubstituted p-tert-butylthiacalix[4]arenes. <b>2023</b> , 29,	O
47	Electrophilicity and nucleophilicity scales at different DFT computational levels.	O
46	Corrosion inhibition efficiency and quantum chemical studies of some organic compounds: theoretical evaluation. <b>2023</b> ,	O
45	Investigation of the dual role of acyl phloroglucinols as a new hope for antibacterial and anti-SARS-CoV-2 agents employing integrated in vitro and multi-phase in silico approaches. 1-18	O
44	Electronic structure and stability of a pure sodium alanate clusters Na12Al12H48, and the interstitial space-doped with Ti, C and H atoms, as a promising hydrogen storage system: Density functional theory. <b>2023</b> ,	0
43	Aromatic Clusters and Hydrogen Storage. <b>2023</b> , 16, 2833	O
42	Linear correlation between electronegativity and adsorption energy of hydrated metal ions by carboxyl-functionalized single-walled carbon nanotubes. <b>2023</b> , 25,	O
41	Insights into the crystal structure and computational studies of newly synthesized thiazolopyrimidine derivatives against adenosine receptor (Thermostabilised HUMAN A2a). <b>2023</b> , 1284, 135372	O
40	Synthesis, biological evaluation and theoretical studies of (E)-1-(4-sulfamoyl-phenylethyl)-3-arylidene-5-aryl-1H-pyrrol-2(3H)-ones as human carbonic anhydrase inhibitors. <b>2023</b> , 38,	О
39	DFT and IQA study of substituent effect on the structure, stability, and bonding properties of CX2 singlet and triplet carbenes.	O

38	One-Bond-Nucleophilicity and -Electrophilicity Parameters: An Efficient Ordering System for 1,3-Dipolar Cycloadditions. <b>2023</b> , 145, 7416-7434	O
37	Insights into the Three-Component Coupling Reactions of Aldehydes, Alkynes, and Amines Catalyzed by N-heterocyclic Carbene Silver: A DFT Study. <b>2023</b> , 13, 646	O
36	Efficient Synthesis of Imine-Carboxylic Acid Functionalized Compounds: Single Crystal, Hirshfeld Surface and Quantum Chemical Exploration. <b>2023</b> , 28, 2967	0
35	New azo-azomethine derivatives: Synthesis, characterization, computational, solvatochromic UV-Vis absorption and antibacterial studies. <b>2023</b> , 1284, 135451	O
34	Fractional Charge Density Functional Theory and Its Application to the Electro-inductive Effect. <b>2023</b> , 14, 3329-3334	O
33	Synthesis, X-ray structure, DFT investigation, and molecular docking of 1,3,5-tricyclohexyl-1,3,5-triazinane-2,4,6-trione, a cyclic polyamide with anti HIV-1 (RT), antiplatelet, and anticoagulant activities.	O
32	A Vibrational Spectroscopic Investigation of 2,2'-Bithiophene Using Experimental and DFT Methods.	0
31	Computational investigation of dimethoate and $\mathbb{E}$ yclodextrin inclusion complex: molecular structures, intermolecular interactions, and electronic analysis.	O
30	Transition metal (X = Mn, Fe, Co, Ni, Cu, Zn)-doped graphene as gas sensor for CO2 and NO2 detection: a molecular modeling framework by DFT perspective. <b>2023</b> , 29,	0
29	Synthesis, characterization, and quantum chemistry local chemical reactivity description of new phosphorylated derivatives of piperazine. 1-11	O
28	Corrosion Inhibiting by Some Organic Heterocyclic Inhibitors Through Langmuir Adsorption Mechanism on the Al-X (X = Mg/Ga/Si) Alloy Surface: A Study of Quantum Three-Layer Method of CAM-DFT/ONIOM. <b>2023</b> , 9,	O
27	Computational evaluation on molecular stability and binding affinity of methyldopa against Lysine-specific demethylase 4D Enzyme through quantum chemical computations and molecular docking analysis. <b>2023</b> , 135518	Ο
26	Coating of favipiravir (FVP) on silver nanoparticles: First principle study. 2023,	O
25	Efficient Synthesis, Spectroscopic Characterization, and Nonlinear Optical Properties of Novel Salicylaldehyde-Based Thiosemicarbazones: Experimental and Theoretical Studies. <b>2023</b> , 8, 13982-13992	Ο
24	(MgO)60: A magic cluster active in UV range under DFT study. <b>2023</b> ,	0
23	Study of N -methyl-5-nitroindazolylacrylonitriles as a Function of Quantum Parameters Employing Density Function Theory Methods: Comparative Theoretical Study and Nonlinear Optical Properties. <b>2023</b> , 8,	Ο
22	The role of ETFS amino acids on the stability and inhibition of p53-MDM2 complex of anticancer p53-derivatives peptides: Density functional theory and molecular docking studies. <b>2023</b> , 122, 108472	0
21	Perturbed reactivity descriptors in the grand canonical ensemble.	Ο

20	Electronic effects of the substituted dopants on stability and reactivity of difuranosilapyridine-4-ylidenes: DFT approach.	O
19	Newly designed triazatruxene-based dye-sensitized solar cells containing different benzothiazine Elinkers: Geometric, optoelectronic, charge transfer properties, and cyanoacrylic acid versus benzoic acid. <b>2023</b> , 1224, 114127	O
18	Engineering magic number Au19 and Au20 cage structures using electron withdrawing atoms.	O
17	Covalent Organic Polymer Containing Nitrogen and Oxygen Groups with High Adsorption Capacity and Selectivity for Gold Ions under Strongly Acidic Conditions.	O
16	Effect of confinement and external mechanical force on the cleavage of the bond in a diatomic molecule.	0
15	SYNTHESIS, OPTICAL AND THERMAL ANALYSIS OF p-BROMO CHALCONE DERIVATIVES: A THEORETICAL AND EXPERIMENTAL STUDIES. <b>2023</b> , 135591	O
14	A MEDT study of the mechanism and selectivity of the hetero-DielsAlder reaction between 3-benzoylpyrrolo[1,2-c][1,4]-benzoxazine-1,2,4-trione and vinyl acetate.	О
13	Synthesis, spectral characterization, computational studies, antifungal, DNA interaction, antioxidant and fluorescence property of novel Schiff base ligand and its metal chelates. <b>2023</b> , 122765	O
12	Computational Methods in the Drug Delivery of Carbon Nanocarriers onto Several Compounds in Sarraceniaceae Medicinal Plant as Monkeypox Therapy. <b>2023</b> , 11, 84	О
11	A molecular electron density theory study of mechanism and selectivity of the intramolecular [3+2] cycloaddition reaction of a nitronelinylphosphonate adduct.	О
10	The Relevance of Lithium Salt Solvate Crystals in Superconcentrated Electrolytes in Lithium Batteries. <b>2023</b> , 16, 3700	O
9	Indotricarbocyanine dyes relevant for photodynamic therapy and their radicals: Substituent effects studied by optical and electrochemical methods. <b>2023</b> , 216, 111344	O
8	Adsorption mechanism and removal efficiency of magnetic graphene oxide-chitosan hybrid on aqueous Zn(II). <b>2023</b> , 241, 124588	О
7	A kinetic perspective of charge transfer reactions: the downfall of hard/soft acid/base interactions. <b>2023</b> , 142,	O
6	Tailoring and functionalizing the graphitic-like GaN and GaP nanostructures as selective sensors for NO, NO2, and NH3 adsorbing: a DFT study. <b>2023</b> , 29,	О
5	Magnetic Adsorbent Decorated with Poly(N-Isopropylacrylamide) (PNIPAM) Brushes for the Vortex-Assisted Solid Phase Extraction (VASPE) of Lead in Water, Cigarettes and Soil with High-Resolution Continuum Source Flame Atomic Absorption Spectrometry (HR-CS FAAS)	O
4	Divalent europium-based contrast agents for magnetic resonance imaging. <b>2023</b> ,	О
3	Correlation Between Halogens Atoms Elements, Their Positions on the Main Chain of Organic Compounds, and Corrosion Inhibition Performance. <b>2023</b> , 65-84	O

Synthesis, physico-chemical characterization and theoretical exploration of some 2,4,5-triaryl imidazole derivatives.

О

Dopamine delivery systems based on C60 and C24 with B and N as substituents.

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