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108	Molecular dynamics simulation of model asphaltenes between surfaces of varying polarity. <b>2023</b> , 331, 125842	1
107	Electronic spectroscopy of cationic adamantane clusters and dehydrogenated adamantane in helium droplets. <b>2022</b> , 24, 23142-23151	0
106	Molecular electrostatic potential as a general and versatile indicator for electronic substituent effects: statistical analysis and applications.	O
105	Understanding the performance of graphdiyne membrane for the separation of nitrate ions from aqueous solution at the atomistic scale. <b>2023</b> , 118, 108337	O
104	QM/MM Simulations for the Broken-Symmetry Catalytic Reaction Mechanism of Human Arginase I. <b>2022</b> , 7, 32536-32548	Ο
103	Charged Small Molecule Binding to Membranes in MD Simulations Evaluated against NMR Experiments. <b>2022</b> , 126, 6955-6963	0
102	A Quantum-Guided Molecular Mechanics Force Field for the Ferrocene Scaffold. <b>2022</b> , 87, 12334-12341	O
101	Chirality Discrimination at Binary Organic Water Interfaces Monitored by Interfacial Tension Measurements With Preliminary Comparison With MD Simulations.	0
100	Benchmarking coarse-grained models of organic semiconductors via deep backmapping. 10,	О

99	An Overview of Basis Set Effects for Diatomic Boron Nitride Compounds (B2N(?,0)): A Quantum Symmetry Breaking. <b>2022</b> , 4, 338-350	O
98	Molecular dynamics simulations of interfacial structure, dynamics, and interfacial tension of tetrabutylammonium bromide aqueous solution in the presence of methane and carbon dioxide.	O
97	HYDROGEN ADSORPTION AND STORAGE ON PALLADIUM-FUNCTIONALIZED C20 BOWL AND C20H10 BOWL MOLECULE INCLUDING HYDROGEN SATURATION. <b>2022</b> , 63, 1399-1408	O
96	The Effect of Surface Composition on the Selective Capture of Atmospheric CO2 by ZIF Nanoparticles: The Case of ZIF-8.	2
95	Infrared intensities of $\$(B_{6}C)^{2-}$ a true challenge for DFT methods. <b>2022</b> , 28,	О
94	Analytic High-Order Energy Derivatives for Metal Nanoparticle-Mediated Infrared and Raman Scattering Spectra within the Framework of Quantum Mechanics/Molecular Mechanics Model with Induced Charges and Dipoles.	O
93	Structure of the two-component S-layer of the archaeon Sulfolobus acidocaldarius.	0
92	DFT study of regio- and stereo-selective 13DC reaction between diazopropane and substituted chalcone derivatives: Molecular docking of novel pyrazole derivatives as Anti-Alzheimer Agents.	O
91	Theoretical exploitation of 1,2,3,4,5,6-hexachloro- and 1,2,3,4,5,6-hexafluorocyclohexane isomers as biologically active compounds.	O
90	On the hydrolysis of iron ions: DFT-based molecular dynamics perspective. <b>2022</b> , 367, 120323	O
89	Improving the accuracy of GIPAW chemical shielding calculations with cluster and fragment corrections. <b>2022</b> , 122, 101832	1
88	Conceptual Density Functional Theory. 2022,	O
87	Controlling anisotropic properties by manipulating the orientation of chiral small molecules.	1
86	Why Do Sulfone-Containing Polymer Photocatalysts Work So Well for Sacrificial Hydrogen Evolution from Water?. <b>2022</b> , 144, 19382-19395	2
85	Computational Study of Two Three-Dimensional Co(II)-Based Metal Organic Frameworks as Quercetin Anticancer Drug Carriers.	O
84	Enhancing NO Uptake in Metal-Organic Frameworks via Linker Functionalization. A Multi-Scale Theoretical Study. <b>2022</b> , 4, 1300-1311	1
83	DFT Investigations on the Ring-Opening Polymerization of Trimethylene Carbonate Catalysed by Heterocyclic Nitrogen Bases. <b>2022</b> , 12, 1280	О
82	Theoretical Investigation of Regiodivergent Addition of Anilines and Phenolates to p-Benzoquinone Ring.	O

81	Analytic Linear Vibronic Coupling Method for First-Principles Spin-Dynamics Calculations in Single-Molecule Magnets.	1
80	Cellulose Fast Pyrolysis Activated by Intramolecular Hydrogen Bonds. <b>2022</b> , 126, 7806-7819	O
79	Comparative Study of Natural Dye Sensitized Solar Cells using Inedible Extracts from Kumkum, Kamala and Malabar Spinach Fruits. <b>2022</b> , 114385	O
78	A stability analysis of choline chloride: urea deep eutectic solvent using density functional theory. <b>2022</b> , 1217, 113921	O
77	Electro-osmotic drag coefficient of Nafion membrane with low water Content for Proton exchange membrane fuel cells. <b>2022</b> , 8, 598-612	O
76	New family of Type V eutectic solvents based on 1,10-phenanthroline and their application in metal extraction. <b>2023</b> , 215, 105971	O
75	Apples to apples comparison of standardized to unstandardized principal component analysis of methods that assign partial atomic charges in molecules. <b>2022</b> , 12, 31617-31628	О
74	Influences of electrostatic models on organic crystal structure prediction $\mathbb B$ case study of pentacene.	O
73	Kinetics in DMS: Modeling Clustering and Declustering Reactions.	0
72	Effect of Pressure on the Distribution of Electrons in a Cluster of H2S.	O
71	Structure and Transport Properties of Poly(ethylene oxide)-Based Cross-Linked Polymer Electrolytes-A Molecular Dynamics Simulations Study.	O
70	On the diffusion of ketoprofen and ibuprofen in water: an experimental and theoretical approach. <b>2022</b> , 106955	O
69	Chemical Absorption of CO 2 Enhanced by Solutions of Alkali Hydroxides and Alkoxides at Room Temperature. <b>2022</b> , 7,	O
68	Theoretical speculation on the chemical reaction activity site and degradation mechanism of chloramphenicol. <b>2022</b> , 140195	O
67	Computational and experimental therapeutic efficacy analysis of andrographolide phospholipid complex self-assembled nanoparticles against Neuro2a cells. <b>2022</b> , 130283	1
66	Improving the kinetic resolution of rac-2-(diphenylthiophosphinoferrocene) methanol catalyzed by Thermomyces lanuginosus lipase immobilized on immobead-150. <b>2023</b> , 535, 112867	O
65	Molecular simulation for R1123 thermophysical properties. <b>2022</b> , 36, 96-101	0
64	Multivalent optical cycling centers: towards control of polyatomics with multi-electron degrees of freedom. <b>2022</b> , 25, 154-170	O

63	Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning.	0
62	The effects of the nature of the sterol on the properties and stability of niosome bilayer vesicles. <b>2023</b> , 369, 120811	O
61	para-substituted pyridines: Effects on the interaction with 2-perfluoropropyl iodide and vibrations. <b>2023</b> , 1275, 134632	O
60	DFT and COSMO-RS studies on dicationic ionic liquids (DILs) as potential candidates for CO2 capture: the effects of alkyl side chain length and symmetry in cations. <b>2022</b> , 12, 35418-35435	O
59	IIYCIReaction between Alkynes and Catechol-Thiol Derivatives Prompted by Metal Nanocatalysis: Mechanism Study by DFT Calculation.	O
58	Growing Spicy ONIOMs: Extending and generalizing concepts of ONIOM and many body expansions.	O
57	Towards a rational design of natural deep eutectic solvents for the extraction of polyphenols from Luma apiculata. <b>2022</b> , 121155	О
56	Differentiation of Seven Isomeric n-Pentylquinoline Radical Cations Based on Energy-Resolved Medium-Energy Collision-Activated Dissociation.	O
55	ZIF for CO2 Capture: Structure, Mechanism, Optimization, and Modeling. 2022, 10, 2689	O
54	Computational Characterization of Zr-Oxide MOFs for Adsorption Applications.	O
53	Near-Infrared-Emitting Meso-Substituted Heptamethine Cyanine Dyes: From the Synthesis and Photophysics to Their Use in Bioimaging. <b>2023</b> , 11, 47	O
52	Excitation Energies of Embedded Chromophores from Frozen-Density Embedding Theory Using State-Specific Electron Densities of the Environment. <b>2023</b> , 127, 535-545	O
51	Combined experimental and molecular simulation study of arginine/PBI composite membranes for high-temperature fuel cells. <b>2023</b> , 58, 1523-1537	O
50	Catalytic Oxidation of Benzoins by Hydrogen Peroxide on Nanosized HKUST-1: Influence of Substituents on the Reaction Rates and DFT Modeling of the Reaction Path. <b>2023</b> , 28, 747	1
49	Weak Electrostatic Interactions with Bisphosphine Ligands Facilitate Reductive Elimination of PhCF 3 from Pd(II) Complexes.	O
48	Synthesis and topology analysis of chloridotriphenyl(triphenyl phosphate-D)tin(IV). 2023, 79,	O
47	Green Electrospinning of Biodegradable Cellulose Acetate Nanofibrous Membranes with Tunable Porosity.	О
46	One-electron self-interaction error and its relationship to geometry and higher orbital occupation.	O

45	Diffusion and dynamics of Noble Gases in Hydroquinone Clathrate channels.	0
44	CO2 Dipole Moment: A Simple Model and Its Implications for CO2-Rock Interactions. <b>2023</b> , 13, 87	Ο
43	Drug Repurposing to Inhibit Histamine N-Methyl Transferase. <b>2023</b> , 28, 576	0
42	On the quest for a molecular vibration whose absolute intensity is described solely by fluctuations of atomic dipoles: Can we find it?. <b>2023</b> , 291, 122321	O
41	Origin of Catalysis by Nitroalkane Oxidase. <b>2023</b> , 127, 151-162	0
40	Molecular Structure of 2-hydroxy-5-methyl-2-nitroazobenzene Isomer: DFT Insight.	O
39	NON-COVALENT INTERATOMIC INTERACTIONS IN TETRAFLUORO-SUBSTITUTED ZINC PHTHALOCYANINE. <b>2022</b> , 63, 1923-1928	0
38	Vibrational Spectroscopic Analysis of 1,3-Dianiline Squarate: Infrared, Normal Raman, Surface-Enhanced Raman Scattering, and Density Functional Theory Calculations. <b>2023</b> , 127, 421-428	Ο
37	Transferability of the Electrostatic Parameters of the Polarizable Gaussian Multipole Model.	0
36	Simulation of polymeric mixed ionic and electronic conductors with a combined classical and quantum mechanical model.	1
35	Machine Learning Identification of Active Sites in Graphite-Conjugated Catalysts. 2023, 127, 2303-2313	0
34	Molecular Simulations on the Coalescence of Water-in-Oil Emulsion Droplets with Non-ionic Surfactant and Model Asphaltene.	O
33	Atomic charges in molecules defined by molecular real space partition into atomic subspaces. <b>2023</b> , 25, 9020-9030	0
32	Consequences of Overfitting the van der Waals Radii of Ions. <b>2023</b> , 19, 2064-2074	O
31	Understanding of three different polyvinylpyrrolidone (PVP) based battery binders blends on graphene surfaces from first principles via DFT simulations. <b>2023</b> , 301, 127548	0
30	Electronic structure and detonation property prediction of pentazolate derivatives: Aminopentazole, diaminopentazole cations, azopentazole, and 1,2-diazopentazole. <b>2023</b> , 1285, 135420	O
29	Photophysical and photochemical properties of 3-hydroxyflavone in ethanol solution: Implicit vs explicit solvent models. <b>2023</b> , 381, 121783	О
28	Fragmentation route of doubly ionized benzene, aniline, and nitroanilines monomers using a novel protocol from density functional theory and QTAIM. <b>2023</b> , 29,	0

27	Ion Pairing in Ionic Liquids. <b>2022</b> , 522-535	О
26	Investigation on Gold[ligand Interaction for Complexes from Gold Leaching: A DFT Study. 2023, 28, 1508	O
25	Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study.	0
24	Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. 1-39	O
23	Evaluation of the affinity of asphaltene molecular models A1 and A2 by the water/oil interfaces based on a novel concept of solubility parameter profiles obtained from MD simulations. <b>2023</b> , 376, 121430	0
22	Anticorrosion Effect of Terephthalamide Core: Bis(2-hydroxybenzoic Acid) for Steel in Biogasoline. <b>2023</b> , 37, 4429-4445	О
21	What is the Optimal Dipole Moment for Nonpolarizable Models of Liquids?. 2023, 19, 1790-1804	О
20	Modelling Complex Bimolecular Reactions in a Condensed Phase: The Case of Phosphodiester Hydrolysis. <b>2023</b> , 28, 2152	О
19	Novel Carbon Nanozymes with Enhanced Phosphatasellke Catalytic Activity for Antimicrobial Applications.	О
18	Machine Learning-Aided Discovery of Nanoporous Materials for Energy- and Environmental-Related Applications. <b>2023</b> , 283-318	O
17	Modeling the Effect of Disorder in the Two-Dimensional Electronic Spectroscopy of Poly-3-hexyltiophene in an Organic Photovoltaic Blend: A Combined Quantum/Classical Approach. <b>2023</b> , 127, 6793-6801	О
16	The Solute Polarization and Structural Effects on the Nonlinear Optical Response of Based Chromone Molecules.	О
15	Unraveling Binding Mechanism and Stability of Urease Inhibitors: A QM/MM MD Study. <b>2023</b> , 28, 2697	О
14	Data science enables the development of a new class of chiral phosphoric acid catalysts. 2023,	О
13	Influence of water on the conformations and interactions within two choline chloride-based deep eutectic solvents: a density functional theory investigation.	О
12	Kinetics and Energetics of Electron Transfer to Dimer Radical Cations. <b>2023</b> , 127, 2881-2886	O
11	Solvation Environments in Porous Ionic Liquids Determine Selectivity in CO2 Conversion to Cyclic Carbonates. <b>2023</b> , 127, 3266-3277	O
10	Computational Investigations into Two-Photon Fibril Imaging Using the DANIR-2c Probe. <b>2023</b> , 127, 3119-312	250

9	A unique case of polymorphism in polyiodide networks resulting from the reaction of the drug methimazole and I2.	O
8	Group 4 metal silylidenes and germylidenes: towards the silicon and germanium variations of olefin metathesis. <b>2023</b> , 33, 145-152	O
7	Separation of phenolic compounds from water by using monoterpenoid and fatty acid based hydrophobic deep eutectic solvents. <b>2023</b> , 381, 121806	0
6	A soft co-crystalline solid electrolyte for lithium-ion batteries.	O
5	Population analysis and the effects of Gaussian basis set quality and quantum mechanical approach: main group through heavy element species. 11,	0
4	Structural and Dynamic Characterization of Lilbnic Liquid Electrolyte Solutions for Application in Li-lon Batteries: A Molecular Dynamics Approach. <b>2023</b> , 9, 234	О
3	A Theoretical Study of Tris-(&lt;i&gt;o&lt;/i&gt;-benzoquinonediimine)-First-Row Divalent Transition Metal Complexes. <b>2023</b> , 13, 172-188	0
2	CRAFTED: An exploratory database of simulated adsorption isotherms of metal-organic frameworks. <b>2023</b> , 10,	O
1	Decomposition of triazole and 3-nitrotriazole upon low-energy electron attachment.	О