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264	Theoretical Perspective for the Relationship Between Structures and Luminescent Properties of Red Thermally Activated Delayed Fluorescence Molecules.		1
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Direct assembly between closed-shell coinage metal superatoms. 262 7 Combustion kinetics of n-propylamine: Theoretical calculations and ignition delay time 261 measurements. 2022, 324, 124710 Effect of intermolecular hydrogen bonds on the proton transfer and fluorescence characteristics of 260 O 1?-hydroxy-2?-acetonaphthone. **2022**, 361, 119555 Theoretical study on the mechanism of hot excitons combined with aggregation-induced emission 259 in efficient red fluorescent molecules. Two Novel Co-Crystals of Naproxen: Comparison of Stability, Solubility and Intermolecular 258 Ο Interaction. 2022, 15, 807 Copper oxide modified activated carbon for enhanced adsorption performance of siloxane: An 257 experimental and DFT study. 2022, 154200 Voltage-Dependent Emission Varying from Blue to OrangeRed from a Nondoped Organic 256 Light-Emitting Diode with a Single Emitter. 2022, 12, 2333 Preparation of hierarchically floral ZIF-8 derived carbon@polyaniline@Ni/Al layered double 255 hydroxides composite with outstanding removal phenomenon for saccharin. 2022, 138127 Binary droplet interactions in shear water-in-oil emulsion: A molecular dynamics study. 2022, 119823 254 Deep removal of chlorobenzene based volatile organic compounds from exhaust gas with ionic 253 liquids. 2022, 298, 121610 Photochemical and Molecular Dynamics Studies of Halide Binding in Flavoenzyme Glucose Oxidase. 252 Physical mechanism on Linear Spectrum and Nonlinear Spectrum in double helical carbon 251 nanomoleculeInfinitene. 2022, 121674 Effective absorption of dichloromethane using deep eutectic solvents. 2022, 439, 129666 250 1 Nucleotide Recognition by a Guanidinocalixarene Receptor in Aqueous Solution. 249 O In Search of Preferential Macrocyclic Hosts for Sulfur Mustard Sensing and Recognition: A Computational Investigation through the New Composite Method r2SCAN-3c of the Key Factors 248 \circ Influencing the Host-Guest Interactions, 2022, 12, 2517 Detection of cocoyl sarcosine utilizing an extended-gate-type organic field-effect transistor 247 functionalized with a copper(II)-dipicolylamine complex. Dynamic construction of self-assembled supramolecular H12SubPcB-OPhCOOH/Ag3PO4 S-scheme 246 Ο arrays for visible photocatalytic oxidation of antibiotics. 2022, 121882 Site- and Enantioselective Manganese-Catalyzed Benzylic CH Azidation of Indolines. 2022, 144, 15383-15390 2

244	Palladium-Catalyzed Aryldifluoromethylation of Aryl Halides with Aryldifluoromethyl Trimethylsilanes.	0
243	Constructing Molecular Bridge for High-Efficiency and Stable Perovskite Solar Cells based on P3HT Hole Transport Material.	
242	Physical Mechanisms of Intermolecular Interactions and Cross-Space Charge Transfer in Two-Photon BDBT-TCNB Co-Crystals. 2022 , 12, 2757	0
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240	Complexes of Ce(III) and Bis(pyrazolyl)borate Ligands: Synthesis, Structures, and Luminescence Properties.	O
239	Palladium-Catalyzed Aryldifluoromethylation of Aryl Halides with Aryldifluoromethyl Trimethylsilanes.	
238	Synthesis of Open-Cage Fullerenes Containing a H-Bond between the Encapsulated Water Molecule and the Amide Moiety on the Rim of the Orifice. 2022 , 2022,	
237	Mechanistic Study of Asymmetric Alkynylation of Isatin-Derived Ketimine Mediated by a Copper/Guanidine Catalyst.	
236	Paying Comprehensive Attention to the ESPT Mechanism and Luminescent Property of Salicylic Acid and Its Derivatives in Various Microenvironments. 2200400	0
235	A strategy to design nonlinear optical materials: Self-assembling by ⊞ Batacking.	
234	Theoretical investigation on the sensing mechanism of a fluorescent probe 3TBN for cyanide anion detection. 2022 , 1215, 113837	
233	Exploiting proton masking to protect amino achieve efficient capture CO2 by amino-acids deep eutectic solvents. 2022 , 299, 121787	O
232	Electronic structure calculations of the fundamental interactions in solvent extraction desalination. 2022 , 364, 119986	0
231	Computational design of a chitosan derivative for improving the color stability of anthocyanins: Theoretical calculation and experimental verification. 2022 , 219, 721-729	O
230	Separation of anthracene and carbazole from crude anthracene via imidazolium-based ionic liquids. 2023 , 331, 125704	0
229	Molecular insights into the CO2 separation mechanism of GO supported deep eutectic solvent membrane. 2022 , 366, 120248	O
228	Molecular dynamics simulation of CO2 hydrate growth in salt water. 2022 , 366, 120237	1
227	Theoretical perspective for substitution effect on luminescent properties of through space charge transfer-based thermally activated delayed fluorescence molecules. 2023 , 285, 121899	1

226	Molecular recognition and spectral tuning of organic dyes in water by amide naphthotubes. 2022 , 58, 9413-9416	O
225	Effects of a long-short axis skeleton on the excited-state properties of ultraviolet hot exciton molecules: luminescence mechanism and molecular design. 2022 , 24, 22309-22318	Ο
224	Mechanistic insight into the borrowing-hydrogen N-alkylation catalyzed by an MLC catalyst with dual proton-responsive sites.	O
223	Recyclable rhodium-catalyzed CH activation/[4 + 2] annulation with unconventional regioselectivity at ambient temperature: experimental development and mechanistic insight. 2022 , 24, 7012-7021	О
222	Theoretical insights into the mechanism and origin of chemoselectivity in the catalyst- and directing group-dependent oxidative cyclization of diynes with pyridine N-oxides. 2022 , 9, 5168-5177	O
221	A flexible, sensitive and stable humidity sensor based on an all-polymer nanofiber film. 2023 , 330, 133268	О
220	Anion Photoelectron Spectroscopy and Quantum Chemical Calculations of Bimetallic Oxide Clusters YCu2On (n = 28). 2022, 126, 6067-6079	О
219	Tri-explosophoric groups driven fused energetic heterocycles featuring superior energetic and safety performances outperforms HMX. 2022 , 13,	4
218	Metal-Free Phosphination and Continued Functionalization of Pyridine: A Theoretical Study. 2022 , 27, 5694	1
217	Exploring the Photophysics of a Zn2+ Fluorescence Sensor and Its Sensing Mechanism. 2022 , 126, 6124-6134	0
		U
216	Alkoxy-Substituted Quadrupolar Fluorescent Dyes. 2022 , 144, 16841-16854	0
216	Alkoxy-Substituted Quadrupolar Fluorescent Dyes. 2022, 144, 16841-16854 A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane.	
	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole	0
215	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane. Regiocontrolled Rh(III)-catalyzed C-C coupling/C-N cyclization mediated by distinctive 1,2-migratory	0
215	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane. Regiocontrolled Rh(III)-catalyzed C-C coupling/C-N cyclization mediated by distinctive 1,2-migratory insertion of gem-difluoromethylene allenes: reaction development and mechanistic insight. 2022, 107849	0
215 214 213	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane. Regiocontrolled Rh(III)-catalyzed C-C coupling/C-N cyclization mediated by distinctive 1,2-migratory insertion of gem-difluoromethylene allenes: reaction development and mechanistic insight. 2022, 107849 Iridium-Catalyzed Stereoselective Transfer Hydrogenation of 1,5-Benzodiazepines. 2022, 87, 12001-12018	o o o
215 214 213 212	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane. Regiocontrolled Rh(III)-catalyzed C-C coupling/C-N cyclization mediated by distinctive 1,2-migratory insertion of gem-difluoromethylene allenes: reaction development and mechanistic insight. 2022, 107849 Iridium-Catalyzed Stereoselective Transfer Hydrogenation of 1,5-Benzodiazepines. 2022, 87, 12001-12018 Gold(I)-Catalyzed Tandem Cyclization/Hydroarylation of o-Alkynylphenols with Haloalkynes. Near-infrared fluorophores with absolute aggregation-caused quenching and negligible	000000

208	Insight into the probe BTFMB responses to hydrogen peroxide switching on ESIPT reaction. 2022 , 807, 140067	0
207	Hydrogen bond networks in gas-phase complex anions. 2022 , 12, 29137-29142	O
206	Highly efficient ultralong organic phosphorescence induced by lone pair repulsions and noncovalent interactions.	O
205	Interpenetrating Dye-Functionalized Indium-Organic Frameworks for Photooxidative Cyanation and Oxidative Cyclization.	O
204	26.2: Invited Paper: Computational chemistry study of an aggregation-induced delayed fluorescence material: synthesis and properties. 2022 , 53, 286-299	0
203	Modified Intramolecular-Lock Strategy Enables Efficient Thermally Activated Delayed Fluorescence Emitters for Non-Doped OLEDs.	O
202	Coordination Switch Drives Selective CB Bond Formation by the Non-heme Sulfoxide Synthases.	0
201	Bottom-up design and assembly with superatomic building blocks.	O
200	Theoretical investigation on interface interaction and properties of 3-nitro-1,2,4-triazol-5-one (NTO)/fluoropolymer polymer-bonded explosives (PBXs). 2022 , 141,	0
199	Distinguishing the Quantum Yield and Lifetime of Carbazole-Based Room-Temperature Phosphorescence Materials: QM/MM Study. 2200342	O
198	Coordination Switch Drives Selective CB Bond Formation by the Non-heme Sulfoxide Synthases.	1
197	Anchoring I3Ivia Charge-Transfer Interaction by a Coordination Supramolecular Network Cathode for a High-Performance Aqueous Dual-Ion Battery. 2022 , 14, 47716-47724	2
196	Modified Intramolecular-Lock Strategy Enables Efficient Thermally Activated Delayed Fluorescence Emitters for Non-Doped OLEDs.	1
195	Enantioselective Synthesis of Unnatural Carbamate-Protected ⊞Alkyl Amino Esters via N⊞ Bond Insertion Reactions. 13143-13148	1
194	Comprehensive study on thermal decomposition mechanism and interaction of 3-Nitro-1,2,4-Triazol-5-One/Poly-3-nitromethyl-3-methyloxetane plastic bonded explosives. 2022 , 168, 105753	0
193	Theoretical Investigation on Interactions between N-methylpyrrolidone-FeCl3 and Components in Model Oil: The Role of S-Fe Coordination in Thiophene Removal. 2022 , 120719	O
192	Palladium/PC-Phos-Catalyzed Asymmetric Heck/Tsuji-Trost Reactions of Amino-Tethered 1,3-Cyclohexadiene with Aryl and Alkenyl Halides.	0
191	Palladium/PC-Phos-Catalyzed Asymmetric Heck/Tsuji-Trost Reactions of Amino-Tethered 1,3-Cyclohexadiene with Aryl and Alkenyl Halides.	O

190	Heterologous expression of family GH11 Aspergillus niger xylanase B (AnXylB11) in Pichia pastoris and competitive inhibition by riceXIP: An experimental and simulation study. 2022 , 220, 112907	O
189	Effect of inorganic salt concentration and types on electrophoretic migration of oil droplets in oil-in-water emulsion: A molecular dynamics study. 2022 , 367, 120549	O
188	Experimental and theoretical study on the extraction of keratin from human hair using protic ionic liquids. 2022 , 368, 120626	О
187	Insight into the effect of anions on cycloaddition of CO2 catalyzed by carboxylate anion-based ionic liquids: A theoretical study by QM and MD. 2022 , 368, 120629	O
186	Mechanism analysis and process optimization of acetone than ol azeotrope separation using 1-ethyl-3-methylimidazolium acetate based mixed extractants. 2022 , 379, 134687	0
185	Molecular insight into the polymorphism-dependent organic phosphorescence. 2022 , 208, 110853	O
184	Data-mining based assembly of promising metal-organic frameworks on Xe/Kr separation. 2023 , 304, 122357	0
183	Photostable aggregation-induced emission of iridium(III) complex realizing robust and high-resolution imaging of latent fingerprints. 2023 , 375, 132898	O
182	Phase behavior and molecular insights on the separation of dimethyl carbonate and methanol azeotrope by extractive distillation using deep eutectic solvents. 2023 , 305, 122489	0
181	Extraction-adsorption coupled desulfurization of fuel oil by novel functionalized porous liquids. 2023 , 453, 139935	O
180	Effects of microwave electric field on the structure and association behaviour of asphaltenes: MD and DFT study. 2023 , 265, 118245	0
179	Hydrogen bond network reconstruction of lignite for efficient moisture removal via deep-eutectic-solvent-assisted hydrothermal treatment. 2023 , 334, 126653	O
178	Theoretical Exploration of Peculiar Sandwich-Type Clusters Formed by the Coordination of E92[[E = Si, Ge, Sn) Zintl Clusters: Structural Properties, Active Sites, and Hydrogen Storage.	0
177	Cellulose Regeneration in Imidazolium-Based Ionic Liquids and Antisolvent Mixtures: A Density Functional Theory Study.	O
176	Constructing molecular bridge for high-efficiency and stable perovskite solar cells based on P3HT. 2022 , 13,	3
175	Prominent Spatial Structure and Synergistic Linkage Effects in Bimetallic Titanium Olefin Polymerization Catalysts.	O
174	Alkali-Metal-Free Coinage Metalides: Specific Pairing and Location of Doping Atoms Bring Forth High Stability and Considerable Nonlinear Optical Response.	0
173	Remote Enantioselective [4 + 1] Annulation with Copper-Vinylvinylidene Intermediates.	O

172	Analysis of the structure and chemical bonding of C5H5ScB40: a density functional study. 2022 , 111768	O
171	Mechanistic insight into separation of benzene and cyclohexane by extractive distillation using deep eutectic solvent as entrainer. 2022 , 368, 120780	O
170	Eutectic solvents formed by (+)-DTTA and L-menthol as novel chiral recognition and separation media for enantioselective extraction of valsartan enantiomers. 2022 , 120818	O
169	Rational regulating pore structures of covalent organic frameworks for sulfur hexafluoride capture and separation. 2023 , 306, 122595	O
168	Experimental and theoretical study on efficient CO2 absorption coordinated by molecules and ions of DBN and 1,2,4-triazole formed deep eutectic solvents. 2023 , 334, 126709	1
167	Palladium-catalyzed generation of CO from formic acid for alkoxycarbonylation of internal alkenes exploits a PTSA-assisted NH-Pd mechanism: a DFT mechanistic study.	O
166	Multichannel charge transfer enhanced radiative decay and RISC in TADF materials containing multiple donors and acceptors. 2022 , 10, 18189-18199	O
165	Synthetic perylenequinone as anchoring center of sulfur and catalyst for polysulfides conversion. 2023 , 455, 140847	O
164	Theoretical investigation on intermolecular interactions, co-crystal structure, thermal decomposition mechanism, and shock properties of 3-nitro-1,2,4-triazol-5-one (NTO) and ammonium perchlorate.	O
163	Quantum chemistry insight into the interactions of 1,3-diisopropoxycalix[4]arenecrown-6 with alkali metal cations: Structure, selectivity, and solvation. 2023 , 370, 121054	O
162	Fabrication of a core-shell porphyrin-based magnetic covalent organic framework for effective extraction of PCPs in a wide polarity range. 2023 , 1239, 340615	O
161	Relativistic Modulation of Supramolecular Halogen/Copper Interactions and Phosphorescence in Cu(I) Pyrazolate Cyclotrimers.	O
160	Spodium bonding to anticrown-Hg3 boosts phosphorescence of cyclometalated-PtII complexes.	O
159	A room-temperature formaldehyde sensor based on hematite for breast cancer diagnosis.	O
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157	Facile fabrication of hierarchically porous melamine foam@COF composite for sample treatment of non-targeted food safety analysis and oil/water separation. 2023 , 455, 140900	1
156	Understanding the role of host-guest interactions in enhancing oil recovery through Ecyclodextrin and adamantane modified copolymer. 2023 , 369, 120841	O
155	Adsorption of sulfonamides on polyamide microplastics in an aqueous solution: behavior, structural effects, and its mechanism. 2023 , 454, 140452	O

154	Application of dual-solvent extraction for separating a low-temperature coal tar: A detailed experimental and quantum chemical study. 2023 , 334, 126654	O
153	Revealing self-aggregation mechanism of asphaltenes during oxidative aging using quantum mechanical calculations. 2023 , 371, 121063	O
152	Cyclodextrin as a green anti-agglomerant agent in oil water emulsion containing asphalt. 2023 , 335, 127041	1
151	Anthracene separation from analogous polycyclic aromatic hydrocarbons using the naphthalene-based solvents. 2023 , 335, 127029	O
150	Novel thermo and ion-responsive copolymers based on metallo-base pair directed host-guest complexation for highly selective recognition of Hg2+ in aqueous solution. 2023 , 445, 130610	O
149	Fragmentation modeling of gas-phase ionic liquid clusters in high-voltage electric field. 2023 , 335, 126919	O
148	A DFT Study on the Endo-selectivity Mechanism of Diels-Alder Reaction in Lindenane Dimeric Sesquiterpenes Synthesis Promoted by Pyridines.	O
147	Indirect Control of Donor/Acceptor Interactions for Highly Efficient Space-Confined Thermally Activated Delayed Fluorescence Emitters. 2209708	O
146	The Origin of Stereoselectivity in the Hydrogenation of Oximes Catalyzed by Iridium Complexes: A DFT Mechanistic Study. 2022 , 27, 8349	O
145	Effect of Hydrogen Bond Interaction on the Decomposition Temperature, Aromaticity, and Bond Order of Nonmetallic Pentazolate Salts. 2022 , 22, 7062-7073	2
144	C3-Cyanation of Pyridines: Constraints on Electrophiles and Determinants of Regioselectivity.	2
143	Synergistic Adsorption B hotocatalysis based on Magnetic Metal©rganic Framework Nanoplatforms for Organic Pollutant Removal. 2022 , 5, 18930-18939	O
142	Hierarchically Organized Cocrystal of Tetra-Anionic Porphyrin and Di-Cationic Viologen: Ion Conformations, Supramolecule Interactions, and Porphyrin Arrays.	O
141	A theoretical study on the effects of intramolecular and intermolecular interactions on excited state properties of two NIR-TADF combined with AIE molecules. 2022 , 114000	O
140	Probing into complexation and separation of chiral-at-uranium complex to chiral sulfur enantiomers R/S-ethiproles.	O
139	Photoliquefiable Azobenzene Surfactants toward Solar Thermal Fuels that Upgrade Photon Energy Storage via Molecular Design. 2206623	O
138	Sensitivity and Weak Interaction of Energetic Ionic Salts: An Example Case of C4N18H2.	О
137	C3-Cyanation of Pyridines: Constraints on Electrophiles and Determinants of Regioselectivity.	Ο

136	Accurate geometry and non-covalent interactions in 1-phenylethanol and its monohydrate: A rotational study.	0
135	The intermolecular interactions of ammonia with chlorine and bromine oxides: a theoretical study. 2023 , 29,	O
134	Theoretical and experimental exploration for efficient separation of carbazole from anthracene oil with quaternary ammonium salts via forming deep eutectic solvents. 2022 , 368, 120831	0
133	Phase Equilibria and Mechanism Insights into the Separation of Isopropyl Acetate and Methanol by Deep Eutectic Solvents.	O
132	Boosting Laser-Ignited Combustion Performance of Energetic Materials with Low Sensitivity: Integration of Triazene-Bridged Triazole with Oxygen-Rich Moieties via Noncovalent Self-Assembly.	0
131	Regulating the melting point by non-covalent interaction toward a promising insensitive melt-castable energetic material: 1,2-difluoro-4,5-dinitrobenzene. 2022 , 100002	Ο
130	Physicochemical properties and intermolecular interactions of a novel diacylglycerol oil oleogel made with ethyl cellulose as affected by Ebryzanol. 2023 , 108484	Ο
129	Transport properties of GNR-C60 single-molecule devices.	O
128	Luminescence lifetime tuning of non-conjugated organic clusters through external heavy-atom effect for smartphone-based time-resolved imaging. 2023 , 141452	Ο
127	Density Functional Study of transition metal (Fe,Co,Ni) doped C60 fullerenes as 6-thioguanine delivery system.	Ο
126	Pagoda[n]arenes (n = 4, 5): Extremely Strong Binders for the Tropylium Cation.	Ο
125	Computational investigation of interaction of a cycloplatinated thiosemicarbazone as antitumor and antiparasitic agents with B12N12 nano-cage. 2023 , 5, 100768	Ο
124	Multiple Pathways for Dissociative Adsorption of SiCl4 on the Si(100)-c(42) Surface. 2023 , 15, 213	Ο
123	Stepwise Hydrations of Anhydride Tuned by Hydrogen Bonds: Rotational Study on Maleic Anhydride-(H2O)1-3.	Ο
122	Spiral donor-based host materials for highly efficient blue thermally activated delayed fluorescence OLEDs. 2023 , 458, 141416	Ο
121	Quantum mechanics/molecular mechanics studies on the photoprotection mechanisms of three chalcones. 2023 , 372, 121165	Ο
120	Synergistic effect of hydrogen bonding and Interaction for enhanced adsorption of rhodamine B from water using corn straw biochar. 2023 , 320, 121060	0
119	Enhanced cadmium removal by biochar and iron oxides composite: Material interactions and pore structure. 2023 , 330, 117136	0

118	Promoting intense mechanoluminescence by strengthening C-H?IInteractions in thioxanthene derivatives. 2023 , 211, 111054	O
117	Performance enhancement in thermally activated delayed fluorescence emitters by multi-fold layout. 2023 , 212, 111104	O
116	Application of facilitated transfer mechanisms of SEBS/[P(14)666][TMPP] composite membrane on CH4/N2 separation. 2023 , 11, 109243	O
115	Electrophoretic coalescence behavior of oil droplets in oil-in-water emulsions containing SDS under DC electric field: A molecular dynamics study. 2023 , 338, 127258	O
114	Hyperbranched polyethyleneimine-functionalised chitosan aerogel for highly efficient removal of melanoidins from wastewater. 2023 , 447, 130731	O
113	Novel Strategy of Polymers in Combination with Silica Particles for Reversible Control of Oil W ater Interface. 2023 , 15, 2216-2227	O
112	Mechanism of a Dually Catalyzed Enantioselective Oxa-PictetBpengler Reaction and the Development of a Stereodivergent Variant. 2240-2249	O
111	Construction of Fluorinated Propane-Trap in Metal-Organic Frameworks for Record Polymer-grade Propylene Production under High Humidity Conditions. 2207955	O
110	Anion photoelectron spectroscopy and quantum chemical calculations of bimetallic niobium-aluminum clusters NbAln?/0 (n = 3-12): Identification of half-encapsulated symmetric structure for NbAl12?.	0
109	Special structural and dynamical interplay of cyano-based novel deep eutectic solvent.	O
108	Selective and Efficient Synthesis of Pine Sterol Esters Catalyzed by Deep Eutectic Solvent. 2023 , 28, 993	O
107	CO2 and Magnetic Dual-Responsive Microspheres That Reversibly and Selectively Capture Target Proteins under Mild Conditions. 2023 , 5, 1135-1144	O
106	Open-Cage Fullerene as a Selective Molecular Trap for LiF/[BeF]+.	O
105	A fluoride-free siliceous STW-type zeolite synthesized using a designed organic structure-directing agent. 2023 , 59, 1649-1652	O
104	Theoretical exploration of noncovalent interactions in Sc2C2@C2n ($n = 40, 41, and 42$)?[12]CPP, PF[12]CPP. 2023 , 13, 4553-4563	O
103	Electronic manipulating in hydrated electron simulation of the carbon-halogen bond reductive cleavage.	O
102	Assembly Rules and Dehydration Mechanism of an Unconventional Hydrate: On the Complexity of the Hydrates of Creatine Phosphate Sodium.	0
101	Reduction-Activatable Fluorogenic Nanobody for Targeted and Low-Background Bioimaging. 2023 , 95, 2804-2811	O

100	Helical Trilayer Nanographenes with Tunable Interlayer Overlaps. 2023 , 145, 2815-2821	0
99	Definition of The Tetrel Bond.	1
98	Insight into the Varying Reactivity of Different Catalysts for CO2 Cycloaddition into Styrene Oxide: An Experimental and DFT Study. 2023 , 24, 2123	0
97	Dissecting amide-I vibrations in histidine dipeptide. 2023 , 292, 122424	O
96	Computational approach to understanding the structures, properties, and supramolecular chemistry of pagoda[n]arenes. 2023 , 1281, 135073	0
95	Why does the cyclic pentazolate anion fail to undergo N-oxidization in oxone solution?. 2023 , 47, 5616-5620	O
94	Accelerated screening and assembly of promising MOFs with open Cu sites for isobutene/isobutane separation using a data-driven approach. 2023 , 25, 8608-8623	0
93	Effects of aggregation on the structures and excited-state absorption for zinc phthalocyanine. 2023 , 25, 10278-10287	O
92	Modulation of chiral spectral deflection by van der Waals force-induced molecular electropolarization in catenane oligomers. 2023 , 13, 11055-11061	0
91	Visualization Analysis of Weak Interactions in Chemical Systems. 2023 ,	O
90	Exploring Au(I) Involving Halogen Bonding with N-Heterocyclic Carbene Au(I) Aryl Complexes in Crystalline Media.	0
89	DFT-based Analysis of Siderophore-Metal Ion Interaction for Efficient Heavy Metal Remediation.	O
88	Unveiling the thermodynamic and molecular mechanisms for the separation of diethoxymethane and ethanol azeotrope by deep eutectic solvents. 2023 , 376, 121451	0
87	Theoretical exploration of the mechanisms on the iron complexes catalyzed ammonia borane dehydrogenation and polyaminoborane formation. 2023 ,	O
86	Tuning Solid-State Emission of 9-Anthraldehyde through Cocrystal Engineering. 2023, 13, 595	O
85	Enhanced NH3 permeation of bis[3-(trimethoxysilyl)propyl] amine membranes via coordination with metals. 2023 , 121665	O
84	Exploring the deagglomerating behaviors of selected additives on oxidized asphaltenes using the steered molecular dynamics approach. 2023 , 375, 121327	0
83	Soil amended with Algal Biochar Reduces Mobility of deicing salt contaminants in the environment: An atomistic insight. 2023 , 323, 138172	O

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82	Toward high-performance associative extraction by forming deep eutectic solvent: A component pairing and mechanism study. 2023 , 272, 118602	O
81	One-pot production of 5-methylfurfural (5-MF) and enhanced dewaterability of waste activated sludge by hydrothermal treatment with natural deep eutectic solvents (NADES): Experimental and theoretical studies. 2023 , 464, 142575	O
80	A range of bifunctional vermiculite-based adsorbents for simultaneous removal of Congo red and permanganate. 2023 , 665, 131280	0
79	Recovery of chlorogenic acid from the DES-based extract of Eucommia ulmoides leaves by molecularly imprinted solid-phase extraction. 2023 , 195, 116406	O
78	Lactam node as a two-fold functional unit for achieving highly efficient and tunable dual-state emitters. 2023 , 213, 111198	О
77	Analysis of the dissolution behavior and solubility of Rotigotine form II in different mono-solvents. 2023 , 377, 121532	0
76	Preparation of the starch-lipid complexes by ultrasound treatment: Exploring the interactions using molecular docking. 2023 , 237, 124187	0
75	FeN4-embedded warped nanographene as a potential candidate for scavenging and detecting sulfur-based gases: A DFT study. 2023 , 11, 109705	Ο
74	Oxygen-containing functional groups enhance uranium adsorption by aged polystyrene microplastics: Experimental and theoretical perspectives. 2023 , 465, 142730	0
73	Oxidative desulfurization of thiophene derivatives with L-proline/benzene sulfonic acid deep eutectic solvent and their interaction: An experimental and computational study. 2023 , 406, 136878	O
72	Carbon composites for rapid and effective photodegradation of 4-halogenophenols: characterization, removal performance, and computational studies. 2023 , 441, 114753	O
71	Quantitative analysis of atomic contribution to interaction and phase equilibrium experiment dominated the process design for ternary multi-azeotropic system. 2023 , 571, 113807	O
70	The immobilization of Sr(ll) and Co(ll) via magnetic easy-separation organophosphonate-hydroxyapatite hybrid nanoparticles. 2023 , 315, 123750	O
69	Atomically dispersed nano Au clusters stabilized by Zr on the TS-1 surface: Significant enhancement of catalytic oxidation ability using H2 and O2. 2023 , 619, 156733	O
68	Prolonging oxidation stability of peony (Paeonia suffruticosa Andr.) seed oil by endogenous lipid concomitants: Phospholipids enhance antioxidant capacity by improving the function of tocopherol. 2023 , 197, 116552	0
67	Electrocatalytic hydrogen evolution on the MoS2/C60 heterostructure: Reaction mechanism and activity improvement. 2023 , 624, 157163	O
66	Theoretical study on the influence of the extra N in transition metal-N4 embedded graphene as efficient CO2 reduction catalysts. 2023 , 616, 156494	О
65	A Two-Dimensional Porphyrin Coordination Supramolecular Network Cathode for High-Performance Aqueous Dual-Ion Battery. 2023 , 135,	O

64	A Two-Dimensional Porphyrin Coordination Supramolecular Network Cathode for High-Performance Aqueous Dual-Ion Battery. 2023 , 62,	О
63	Open-Cage Fullerene as a Selective Molecular Trap for LiF/[BeF] +. 2023 , 135,	О
62	Study and Applications of Tetrasubstituted Hypervalent Selenium Halogen Species in Catalytic Electrophilic Halogenations. 2023 , 13, 2386-2395	0
61	Absorption of dichloromethane in deep eutectic solvents: Experimental and computational thermodynamics. 2023 , 311, 123281	O
60	Highly selective extraction of aromatics from aliphatics using an N -methylpyrrolidone-based protic ionic liquid.	O
59	Neutral Monodentate and Hypervalent Chalcogen Bond Catalysis on the Intramolecular Rauhut-Currier Reaction of Bis(enones): A DFT Study.	О
58	Absorption of ethylene dichloride with imidazolium-based ionic liquids. 2023 , 376, 121449	0
57	Mechanistic insights into catalyst-dependent divergent cycloaddition reactions via discrimination between diazo compounds. 2023 , 10, 1606-1616	О
56	Characterization of the interaction between boscalid and tannic acid and its effect on the antioxidant properties of tannic acid. 2023 , 88, 1325-1335	0
55	A Spiro Phosphamide Catalyzed Enantioselective Proton Transfer of Ylides in a Free Carbene Insertion into NH Bonds. 2023 , 62,	O
54	A Spiro Phosphamide Catalyzed Enantioselective Proton Transfer of Ylides in a Free Carbene Insertion into NH Bonds. 2023 , 135,	0
53	Complexation between rice starch and cellulose nanocrystal from black tea residues: Gelatinization properties and digestibility in vitro. 2023 , 234, 123695	O
52	Nano-deterioration of steel passivation film: chloride attack in material defects. 2023, 56,	1
51	Super stable, highly ion-conductive and transparent eutecto-/hydro-gel promotes wearable electronic and visual strain sensing. 2023 , 461, 141965	o
50	AIEgens/Mitochondria Nanohybrids as Bioactive Microwave Sensitizers for Non-Thermal Microwave Cancer Therapy. 2202907	0
49	Highly Efficient Purely Organic Phosphorescence Light-Emitting Diodes Employing a Donor Acceptor Skeleton with a Phenoxaselenine Donor. 2207003	o
48	Weak Interactions Initiate Cℍ and Cជ Bond Dissociation of Ethane on Nb n + Clusters.	0
47	Molecular Dynamics Simulation of CO2 Hydrate Growth in NaCl Aqueous Solution. 2023 , 1-7	O

46	Theoretically Revealing the Response of Intermolecular Vibration Energy Transfer and Decomposition Process of the DNTF System to Electric Fields Using Two-Dimensional Infrared Spectra. 2023 , 24, 4352	O
45	Insights into the regioselectivity and diastereoselectivity of the Nazarov cyclization of 3-alkenyl-2-indolylmethanol with tryptophol. 2023 , 10, 1721-1730	О
44	Reactivity and Selectivity of the DielsAlder Reaction of Anthracene in [Pd6L4]12+ Supramolecular Cages: A Computational Study. 2023 , 62, 4330-4340	O
43	Molecular Insights into CyclodextrinAdamantane-Modified Copolymer Host \(\Gamma\) uest Interactions. 2023 , 39, 3619-3627	О
42	Afterglow OLEDs incorporating bright closely stacked molecular dimers with ultra-long thermally activated delayed fluorescence. 2023 , 6, 1231-1248	0
41	Mechanistic insights into H3BENMeH2 dehydrogenation by Co-based complexes: a DFT perspective. 2023 , 47, 6661-6672	O
40	Activation of metal-involved halogen bonds and classical halogen bonds in gold(i) catalysis. 2023 , 52, 4517-4525	0
39	Tunable Fluorescent Artificial Receptor Biosensor Based on Programmable Lanthanide Metal-Organic Framework for Highly Selective Neurotransmitter Detection. 2300309	О
38	Theoretical insights into luminescence mechanism of Naphthyridine-based thermally activated delayed fluorescence emitter with aggregation-induced emission. 2023 , 817, 140407	O
37	Bis(perfluoroaryl)chalcolanes ArF2Ch (Ch = S, Se, Te) as ÆHole Donors for Supramolecular Applications Based on Noncovalent Bonding. 2023 , 23, 2593-2601	O
36	Selective separation of pyrene from mixed polycyclic aromatic hydrocarbons by a hexahedral metal-organic cage. 2023 , 108326	O
35	Smart Reversible Transformations between Chiral Superstructures of Copper Clusters for Optical and Chiroptical Switching. 2023 , 145, 6166-6176	o
34	Theoretical study on the solvent-free self-catalyzed coupling mechanism of a chiral vicinal diamine and isobutyraldehyde mediated by the outgrowth H 2 O. 2023 , 8,	0
33	Two-photon fluorescence imaging and specifically biosensing of norepinephrine on a 100-ms timescale. 2023 , 14,	o
32	Regulating through space charge transfer in thermally activated delayed fluorescence molecules via donor architectures: theoretical perspective and molecular design. 2023 , 25, 10977-10990	O
31	Stereospecific Nickel-Catalyzed Cross-Electrophile Coupling Reaction of Alkyl Mesylates and Allylic Difluorides to Access Enantioenriched Vinyl Fluoride-Substituted Cyclopropanes. 2023 , 13, 4488-4499	O
30	Roles of Molecular Spatial Arrangement in Exciton Energy Transfer in Organic Light-Emitting Diodes: A Theoretical Study. 2023 , 127, 5950-5957	0
29	Enantioselective Photochemical Carbene Insertion into CII and CII Bonds of 1,3-Diketones by a Guanidine-Amide Organocatalyst. 2023 , 13, 4656-4666	O

28	Role of Non-Covalent Interactions in Carbonic Anhydrase Illiopiramate Complex Based on QM/MM Approach. 2023 , 16, 479	O
27	Mechano-/seeding-triggered crystal-to-crystal phase transition in luminescent switching cocrystals. 2023 , 215, 111275	Ο
26	Chiral discrimination of cyclodecapeptide to anti-COVID-19 clinical candidates: a theoretical study.	0
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23	Co-Solvent Engineering Contributing to Achieve High-Performance Perovskite Solar Cells and Modules Based on Anti-Solvent Free Technology.	O
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20	New insight into atomic-level interpretation of interactions in molecules and reacting systems.	0
19	Crystalline matrix-activated spin-forbidden transitions of engineered organic crystals.	O
18	Highly Hydrophilic ZIF-8 as a Carbonic Anhydrase Mimetic Catalyst for Promoting CO2 Absorption. 2023 , 127, 7184-7196	0
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15	Enhancement of Organic Oxygen Atoms on Metal Cobalt for Sulfur Adsorption and Catalytic Polysulfide Conversion.	O
14	Theoretical investigation of Aryl/Alkyl halide reduction with hydrated electrons from energy and AIMD aspects. 2023 , 29,	0
13	Non-covalent interactions in polymorphs of urea under pressure. 2023 , 142,	O
12	Oxidization enhances type I ROS generation of AIE-active zwitterionic photosensitizers for photodynamic killing of drug-resistant bacteria.	0
11	Prediction, Application, and Mechanism Exploration of Liquid Liquid Equilibrium Data in the Extraction of Aromatics Using Sulfolane. 2023 , 11, 1228	O

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	In situ growth of NH2-MIL-101 metal organic frameworks on biochar for glyphosate adsorption.	
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