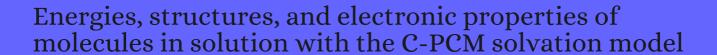
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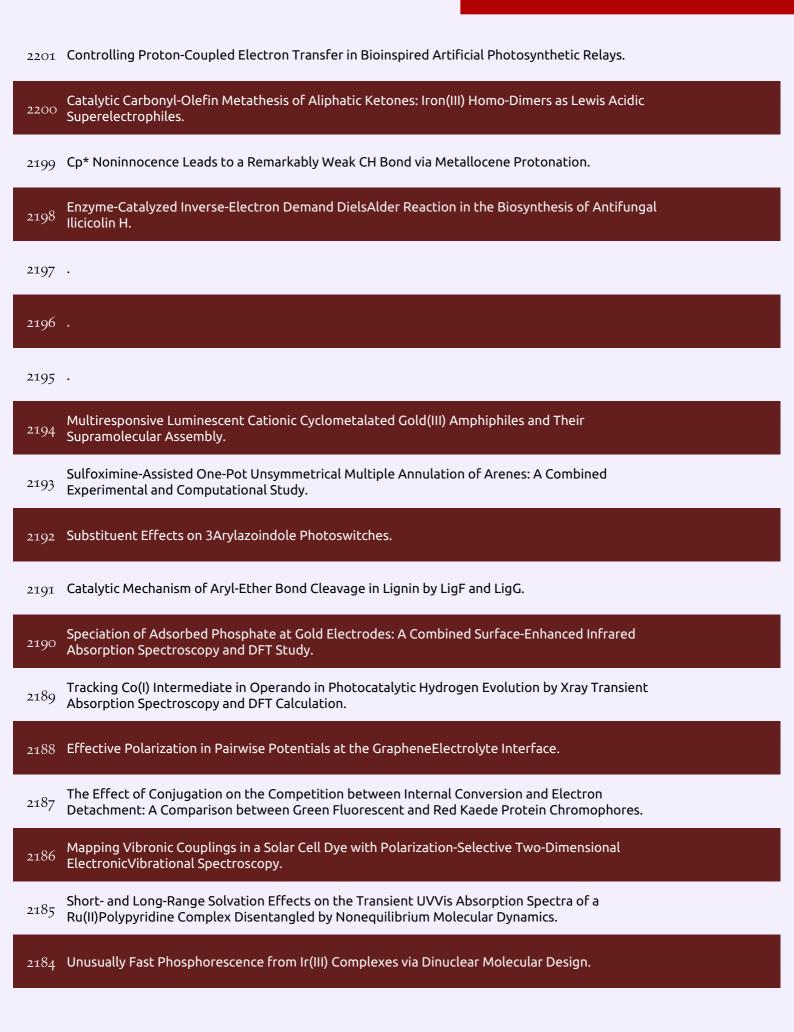
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121	A non expected alternative Ni(0) Species in the Ni-Catalytic Aldehyde and Alcohol Arylation Reactions Facilitated by a 1,5-Diaza-3,7-diphosphacyclooctane Ligand.	0
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119	Ruthenium Azobis (benzothiazole): Electronic Structure and Impact of Substituents on the Electrocatalytic Single-Site Water Oxidation Process.	О
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26	Theoretical studies on the mechanism of molybdenum-catalysed deoxydehydration of diols.	O
25	Computational investigation of dimethoate and <code>tyclodextrin</code> inclusion complex: molecular structures, intermolecular interactions, and electronic analysis.	O
24	(3+2)-Cyclization reactions of unsaturated phosphonites with aldehydes and thioketones.	O

23	New insights into the mechanism of synergetic photoredox/copper(i)-catalyzed carbocyanation of 1,3-dienes: a DFT study.	О
22	Iminium substituent directs cyanide and hydride additions to triiron vinyliminium complexes.	O
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20	Calculation of Excited State Internal Conversion Rate Constant Using the One-Effective Mode Marcus-Jortner-Levich Theory.	O
19	Protodemetalation of (Bipyridyl)Ni(II)Aryl Complexes Shows Evidence for Five-, Six-, and Seven-Membered Cyclic Pathways.	О
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16	Reactivity Factors in Catalytic Methanogenesis and Their Tuning upon Coenzyme F430 Biosynthesis.	O
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14	Evidence of a Wheland Intermediate in Carboxylate-Assisted C(sp2)田 Activation by Pd(IV) Active Catalyst Species Studied via DFT Calculations. 2023 , 13, 724	О
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10	Synthesis, spectroscopic characterization and solid-state electrical behavior of [Ni(L)2] [L = 1,2-di(4-methoxyphenyl)ethene-1,2-dithiolate]: a computational investigation on UVIIis-NIR absorption and electrical transport. 1-12	O
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8	Concerted Proton-Coupled Electron Transfer to a Graphite Adsorbed Metalloporphyrin Occurs by Band to Bond Electron Redistribution.	O
7	SophosQM: Accurate Binding Affinity Prediction in Compound Optimization.	O
6	A Theoretical Study of Tris-(<i>o</i>-benzoquinonediimine)-First-Row Divalent Transition Metal Complexes. 2023 , 13, 172-188	O

5	Regiodivergent Nucleophilic Fluorination under Hydrogen Bonding Catalysis: A Computational and Experimental Study.	Ο
4	Investigation of the solvent effect, regioselectivity, and the mechanism of the cycloaddition reaction between 2-chlorobenzimidazole and benzonitrile oxide.	O
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