

Xin Wang

List of Publications by Year in descending order

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18
papers

509
citations

840776

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h-index

794594

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docs citations

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times ranked

573
citing authors

#	ARTICLE	IF	CITATIONS
1	QM/MM investigation of the catalytic mechanism of processive endoglucanase Cel9G from <i>Clostridium cellulovorans</i> . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11919-11930.	2.8	1
2	Molecular dynamic simulation of prenucleation of apatite at a type I collagen template: ion association and mineralization control. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11370-11381.	2.8	4
3	Trace mild acid-catalysed Z to E isomerization of norbornene-fused stilbene derivatives: intelligent chiral molecular photoswitches with controllable self-recovery. <i>Chemical Science</i> , 2021, 12, 2614-2622.	7.4	12
4	Regiodivergent Intramolecular Nucleophilic Addition of Ketimines for the Diverse Synthesis of Azacycles. <i>Angewandte Chemie</i> , 2020, 132, 1651-1660.	2.0	1
5	Regiodivergent Intramolecular Nucleophilic Addition of Ketimines for the Diverse Synthesis of Azacycles. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 1634-1643.	13.8	31
6	Direct electrochemical defluorinative carboxylation of CF_3 alkenes with carbon dioxide. <i>Chemical Science</i> , 2020, 11, 10414-10420.	7.4	83
7	Molecular docking and molecular dynamics simulation studies on the adsorption/desorption behavior of bone morphogenetic protein-7 on the H_2 -tricalcium phosphate surface. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16747-16759.	2.8	5
8	Molecular dynamics exploration of the amorphous surface structures and properties of the biomimetic H_2 -tricalcium phosphate. <i>Applied Surface Science</i> , 2019, 484, 72-82.	6.1	6
9	Molecular Dynamics Exploration of Ordered-to-Disordered Surface Structures of Biomimetic Hydroxyapatite Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6691-6703.	3.1	12
10	A theoretical study of molecular structure, optical properties and bond activation of energetic compound FOX-7 under intense electric fields. <i>Chemical Physics</i> , 2017, 483-484, 122-131.	1.9	10
11	A theoretical investigation of the competition between hydrogen bonding and lone pair interaction in complexes of TNT with NH_3 . <i>Computational and Theoretical Chemistry</i> , 2015, 1064, 25-34.	2.5	13
12	Theoretical investigations on electronic and charge transport properties of novel organic semiconductors with Triisopropylsilylethynyl (TIPS)-functionalized anthradifuran and anthradithiophene derivatives. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 107-117.	2.5	9
13	Highly Efficient Water-Free Catalyst-Free Nucleophilic Addition Reactions Using Difluoroenoxyasilanes: Dramatic Fluorine Effects. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9512-9516.	13.8	156
14	A BINOL-based ratiometric fluorescent sensor for Zn^{2+} and in situ generated ensemble for selective recognition of histidine in aqueous solution. <i>Analyst</i> , 2013, 138, 5762.	3.5	32
15	Strong lone pair interactions between amine and tri-s-triazine derivatives: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2013, 1017, 144-152.	2.5	7
16	A Catalyst-Free, One-Pot Three-Component Aminomethylation of H_2 -Substituted Nitroacetates: Theoretical and Experimental Studies into the Rate-Accelerating Effects of the Solvent Methanol. <i>Chemistry - an Asian Journal</i> , 2013, 8, 877-882.	3.3	14
17	Dipole polarizabilities of noble gas endohedral fullerenes. <i>Chemical Physics Letters</i> , 2008, 456, 223-226.	2.6	50
18	A G3B3 study of N_4H_4 isomers. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 207-210.	1.5	16