Zhiyu Xue

List of Publications by Year in descending order

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15 papers	143 citations	1307594 7 h-index	1281871 11 g-index
15 all docs	15 docs citations	15 times ranked	115 citing authors

#	Article	IF	Citations
1	CO2 mineralization and CH4 effective recovery in orthoclase slit by molecular simulation. Chemical Engineering Journal, 2022, 430, 133056.	12.7	5
2	Correction of gas adsorption capacity in quartz nanoslit and its application in recovering shale gas resources by CO2 injection: A molecular simulation. Energy, 2022, 240, 122789.	8.8	9
3	Molecular dynamic simulation of prenucleation of apatite at a type I collagen template: ion association and mineralization control. Physical Chemistry Chemical Physics, 2022, 24, 11370-11381.	2.8	4
4	Molecular Dynamics Exploration of the Growth Mechanism of Hydroxyapatite Nanoparticles Regulated by Glutamic Acid. Journal of Physical Chemistry B, 2021, 125, 5078-5088.	2.6	6
5	Molecular Dynamics Characterization of Sr-Doped Biomimetic Hydroxyapatite Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 19704-19715.	3.1	6
6	How Charged Amino Acids Regulate Nucleation of Biomimetic Hydroxyapatite Nanoparticles on the Surface of Collagen Mimetic Peptides: Molecular Dynamics and Free Energy Investigations. Crystal Growth and Design, 2020, 20, 4561-4572.	3.0	15
7	Molecular docking and molecular dynamics simulation studies on the adsorption/desorption behavior of bone morphogenetic protein-7 on the Î²-tricalcium phosphate surface. Physical Chemistry Chemical Physics, 2020, 22, 16747-16759.	2.8	5
8	Effect of Hydroxyapatite Surface on BMP-2 Biological Properties by Docking and Molecular Simulation Approaches. Journal of Physical Chemistry B, 2019, 123, 3372-3382.	2.6	22
9	Molecular dynamics exploration of the amorphous surface structures and properties of the biomimetic Î²-tricalcium phosphate. Applied Surface Science, 2019, 484, 72-82.	6.1	6
10	Nucleation of Biomimetic Hydroxyapatite Nanoparticles on the Surface of Type I Collagen: Molecular Dynamics Investigations. Journal of Physical Chemistry C, 2019, 123, 2533-2543.	3.1	22
11	Molecular Dynamics Exploration of Ordered-to-Disordered Surface Structures of Biomimetic Hydroxyapatite Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 6691-6703.	3.1	12
12	Quantum chemical exploration on the metabolic mechanisms of caffeine by flavin-containing monooxygenase. Tetrahedron, 2016, 72, 2858-2867.	1.9	8
13	Theoretical elucidation of the metabolic mechanisms of phenothiazine neuroleptic chlorpromazine catalyzed by cytochrome P450 isoenzyme 1A2. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	6
14	Theoretical study on the metabolic mechanisms of levmepromazine by cytochrome P450. Journal of Molecular Modeling, 2016, 22, 237.	1.8	4
15	Theoretical study on the N-demethylation mechanism of theobromine catalyzed by P450 isoenzyme 1A2. Journal of Molecular Graphics and Modelling, 2015, 61, 123-132.	2.4	13