

Farideh Badalkhani-Khamseh

List of Publications by Year in descending order

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Version: 2024-02-01

10
papers

180
citations

1163117

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1372567

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85
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploration of phosphorene as doxorubicin nanocarrier: An atomistic view from DFT calculations and MD simulations. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 215, 112513.	5.0	13
2	Heteroatom-containing phosphoramides as carbon steel corrosion inhibitors: Density functional theory and molecular dynamics simulations. <i>Chemical Physics Impact</i> , 2022, 5, 100099.	3.5	12
3	PAMAM and polyester dendrimers as favipiravir nanocarriers: a comparative study using DFT method. <i>Journal of Nanoparticle Research</i> , 2021, 23, 231.	1.9	19
4	Evaluation of BLG ability for binding to 5-FU and Irinotecan simultaneously under acidic condition: A spectroscopic, molecular docking and molecular dynamic simulation study. <i>Journal of Molecular Liquids</i> , 2021, 344, 117758.	4.9	10
5	Theoretical study on the Al-doped biphenylene nanosheets as NO sensors. <i>Chemical Physics Letters</i> , 2020, 754, 137712.	2.6	27
6	Adsorption behavior of pristine, Al-, and Si-doped carbon nanotubes upon 5-fluorouracil. <i>Chemical Physics Letters</i> , 2020, 750, 137492.	2.6	26
7	Influence of dendrimer surface chemistry and pH on the binding and release pattern of chalcone studied by molecular dynamics simulations. <i>Journal of Molecular Recognition</i> , 2019, 32, e2757.	2.1	26
8	Complexation of nicotinic acid with first generation poly(amidoamine) dendrimers: A microscopic view from density functional theory. <i>Chemical Physics Letters</i> , 2017, 684, 103-112.	2.6	23
9	Atomistic computer simulations on multi-loaded PAMAM dendrimers: a comparison of amine- and hydroxyl-terminated dendrimers. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 1097-1111.	2.9	22
10	Effect of methyl groups substitution on the strength of intramolecular hydrogen bonding of naphthazarin: DFT and NBO studies. <i>Journal of the Iranian Chemical Society</i> , 2013, 10, 685-694.	2.2	2