Shikha nangia

List of Publications by Year
in descending order

45 papers	1,972 citations	361413 20 h-index	243625 44 g-index
50 all docs	50 docs citations	50 times ranked	2264 citing authors

#	Article	IF	Citations
1	Adaptive Recombinant Nanoworms from Genetically Encodable Star Amphiphiles. Biomacromolecules, 2022, 23, 863-876.	5.4	4
2	Salt Destabilization of Cationic Colistin Complexation within Polyanionic Microgels. Macromolecules, 2022, 55, 1736-1746.	4.8	4
3	Development of the computational antibiotic screening platform (CLASP) to aid in the discovery of new antibiotics. Soft Matter, 2021, 17, 2725-2736.	2.7	6
4	Persister control by leveraging dormancy associated reduction of antibiotic efflux. PLoS Pathogens, 2021, 17, e1010144.	4.7	10
5	Non-canonical lipoproteins with programmable assembly and architecture. Chemical Communications, 2020, 56, 10281-10284.	4.1	12
6	Molecular mechanism of ultrasound interaction with a blood brain barrier model. Journal of Chemical Physics, 2020, 153, 045104.	3.0	15
7	High-Level Antibiotic Tolerance of a Clinically Isolated Enterococcus faecalis Strain. Applied and Environmental Microbiology, 2020, 87, .	3.1	2
8	Rational identification and characterisation of peptide ligands for targeting polysialic acid. Scientific Reports, 2020, 10, 7697.	3.3	1
9	Interaction of amphiphilic coumarin with DPPC/DPPS lipid bilayer: effects of concentration and alkyl tail length. Physical Chemistry Chemical Physics, 2020, 22, 15197-15207.	2.8	7
10	Predicting selectivity of paracellular pores for biomimetic applications. Molecular Systems Design and Engineering, 2020, 5, 686-696.	3.4	7
11	Paracellular Gatekeeping: What Does It Take for an Ion to Pass Through a Tight Junction Pore?. Langmuir, 2020, 36, 6757-6764.	3.5	10
12	The ghrelin O-acyltransferase structure reveals a catalytic channel for transmembrane hormone acylation. Journal of Biological Chemistry, 2019, 294, 14166-14174.	3.4	26
13	Computational Nanoscopy of Tight Junctions at the Bloodâ€“Brain Barrier Interface. International Journal of Molecular Sciences, 2019, 20, 5583.	4.1	18
14	Obtaining Protein Association Energy Landscape for Integral Membrane Proteins. Journal of Chemical Theory and Computation, 2019, 15, 6444-6455.	5.3	17
15	Palmitoylation of Claudin-5 Proteins Influences Their Lipid Domain Affinity and Tight Junction Assembly at the Bloodâ€“Brain Barrier Interface. Journal of Physical Chemistry B, 2019, 123, 983-993.	2.6	27
16	The Influence of Water on Choline-Based Ionic Liquids. ACS Biomaterials Science and Engineering, 2019, 5, 3645-3653.	5.2	42
17	Dynamics of OmpF Trimer Formation in the Bacterial Outer Membrane ofEscherichia coli. Langmuir, 2018, 34, 5623-5634.	3.5	13
18	Mechanism of Antibacterial Activity of Choline-Based Ionic Liquids (CAGE). ACS Biomaterials Science and Engineering, 2018, 4, 2370-2379.	5.2	94

#	ARTICLE	IF	CITATIONS
19	Development of effective stochastic potential method using random matrix theory for efficient conformational sampling of semiconductor nanoparticles at non-zero temperatures. Journal of Chemical Physics, 2018, 149, 014103.	3.0	7
20	Self-Assembly Simulations of Classic Claudinsâ€"Insights into the Pore Structure, Selectivity, and Higher Order Complexes. Journal of Physical Chemistry B, 2018, 122, 7463-7474.	2.6	37
21	Modeling Diversity in Structures of Bacterial Outer Membrane Lipids. Journal of Chemical Theory and Computation, 2017, 13, 811-824.	5.3	30
22	Architecture of the paracellular channels formed by claudins of the bloodâ€"brain barrier tight junctions. Annals of the New York Academy of Sciences, 2017, 1405, 131-146.	3.8	56
23	Drug-Specific Design of Telodendrimer Architecture for Effective Doxorubicin Encapsulation. Journal of Physical Chemistry B, 2016, 120, 9766-9777.	2.6	13
24	Combinatorial approaches to evaluate nanodiamond uptake and induced cellular fate. Nanotechnology, 2016, 27, 085107.	2.6	19
25	Molecular Architecture of the Blood Brain Barrier Tight Junction Proteinsâ€"A Synergistic Computational and In Vitro Approach. Journal of Physical Chemistry B, 2016, 120, 77-88.	2.6	46
26	Multiscale Approach to Investigate Self-Assembly of Telodendrimer Based Nanocarriers for Anticancer Drug Delivery. Langmuir, 2015, 31, 4270-4280.	3.5	38
27	Signaling Factor Interactions with Polysaccharide Aggregates of Bacterial Biofilms. Langmuir, 2015, 31, 1958-1966.	3.5	4
28	Simulating Gram-Negative Bacterial Outer Membrane: A Coarse Grain Model. Journal of Physical Chemistry B, 2015, 119, 14668-14682.	2.6	69
29	Optical Signature of Formation of Protein Corona in the Firefly Luciferase-CdSe Quantum Dot Complex. Journal of Chemical Theory and Computation, 2014, 10, 5224-5228.	5.3	16
30	A Structureâ€"Property Relationship Study of the Well-Defined Telodendrimers to Improve Hemocompatibility of Nanocarriers for Anticancer Drug Delivery. Langmuir, 2014, 30, 6878-6888.	3.5	16
31	Probing Mechanisms of Bacterial Infection through Molecular Dynamics Simulations. , 2013, , .		0
32	Effects of Nanoparticle Charge and Shape Anisotropy on Translocation through Cell Membranes. Langmuir, 2012, 28, 17666-17671.	3.5	192
33	Theoretical advances in the dissolution studies of mineralâ€"water interfaces. Theoretical Chemistry Accounts, 2010, 127, 271-284.	1.4	13
34	Role of Intrasurface Hydrogen Bonding on Silica Dissolution. Journal of Physical Chemistry C, 2010, 114, 2267-2272.	3.1	13
35	Ab initiostudy of dissolution and precipitation reactions from the edge, kink, and terrace sites of quartz as a function of pH. Molecular Physics, 2009, 107, 831-843.	1.7	35
36	Ab Initio Investigation of Dissolution Mechanisms in Aluminosilicate Minerals. Journal of Physical Chemistry A, 2009, 113, 1343-1352.	2.5	55

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37	Advanced Monte Carlo Approach To Study Evolution of Quartz Surface during the Dissolution Process. Journal of the American Chemical Society, 2009, 131, 9538-9546.	13.7	30
38	Reaction Rates and Dissolution Mechanisms of Quartz as a Function of pH. Journal of Physical Chemistry A, 2008, 112, 2027-2033.	2.5	101
39	Study of a Family of 40 Hydroxylated Î²-Cristobalite Surfaces Using Empirical Potential Energy Functions. Journal of Physical Chemistry C, 2007, 111, 5169-5177.	3.1	30
40	Non-Bornâ^'Oppenheimer Molecular Dynamics. Accounts of Chemical Research, 2006, 39, 101-108.	15.6	197
41	Direct calculation of coupled diabatic potential-energy surfaces for ammonia and mapping of a four-dimensional conical intersection seam. Journal of Chemical Physics, 2006, 124, 124309.	3.0	69
42	Can a Single-Reference Approach Provide a Balanced Description of Ground and Excited States? A Comparison of the Completely Renormalized Equation-of-Motion Coupled-Cluster Method with Multireference Quasidegenerate Perturbation Theory near a Conical Intersection and along a Photodissociation Coordinate in Ammonia. Journal of Physical Chemistry A, 2005, 109, 11643-11646.	2.5	17
43	Army ants algorithm for rare event sampling of delocalized nonadiabatic transitions by trajectory surface hopping and the estimation of sampling errors by the bootstrap method. Journal of Chemical Physics, 2004, 120, 3586-3597.	3.0	74
44	Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Bornâ€"Oppenheimer trajectories. Journal of Chemical Physics, 2004, 121, 7658.	3.0	288
45	Introductory lecture: Nonadiabatic effects in chemical dynamics. Faraday Discussions, 2004, 127, 1.	3.2	190