

Shikha nangia

List of Publications by Year in descending order

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Version: 2024-02-01

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	Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Born–Oppenheimer trajectories. <i>Journal of Chemical Physics</i> , 2004, 121, 7658.	3.0	288
2	Non-Born–Oppenheimer Molecular Dynamics. <i>Accounts of Chemical Research</i> , 2006, 39, 101-108.	15.6	197
3	Effects of Nanoparticle Charge and Shape Anisotropy on Translocation through Cell Membranes. <i>Langmuir</i> , 2012, 28, 17666-17671.	3.5	192
4	Introductory lecture: Nonadiabatic effects in chemical dynamics. <i>Faraday Discussions</i> , 2004, 127, 1.	3.2	190
5	Reaction Rates and Dissolution Mechanisms of Quartz as a Function of pH. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2027-2033.	2.5	101
6	Mechanism of Antibacterial Activity of Choline-Based Ionic Liquids (CAGE). <i>ACS Biomaterials Science and Engineering</i> , 2018, 4, 2370-2379.	5.2	94
7	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. <i>Journal of Chemical Physics</i> , 2004, 120, 3586-3597.	3.0	74
8	Direct calculation of coupled diabatic potential-energy surfaces for ammonia and mapping of a four-dimensional conical intersection seam. <i>Journal of Chemical Physics</i> , 2006, 124, 124309.	3.0	69
9	Simulating Gram-Negative Bacterial Outer Membrane: A Coarse Grain Model. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14668-14682.	2.6	69
10	Architecture of the paracellular channels formed by claudins of the blood–brain barrier tight junctions. <i>Annals of the New York Academy of Sciences</i> , 2017, 1405, 131-146.	3.8	56
11	Ab Initio Investigation of Dissolution Mechanisms in Aluminosilicate Minerals. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1343-1352.	2.5	55
12	Molecular Architecture of the Blood Brain Barrier Tight Junction Proteins—A Synergistic Computational and <i>In Vitro</i> Approach. <i>Journal of Physical Chemistry B</i> , 2016, 120, 77-88.	2.6	46
13	The Influence of Water on Choline-Based Ionic Liquids. <i>ACS Biomaterials Science and Engineering</i> , 2019, 5, 3645-3653.	5.2	42
14	Multiscale Approach to Investigate Self-Assembly of Telodendrimer Based Nanocarriers for Anticancer Drug Delivery. <i>Langmuir</i> , 2015, 31, 4270-4280.	3.5	38
15	Self-Assembly Simulations of Classic Claudins—Insights into the Pore Structure, Selectivity, and Higher Order Complexes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7463-7474.	2.6	37
16	<i>Ab initio</i> study of dissolution and precipitation reactions from the edge, kink, and terrace sites of quartz as a function of pH. <i>Molecular Physics</i> , 2009, 107, 831-843.	1.7	35
17	Study of a Family of 40 Hydroxylated β -Cristobalite Surfaces Using Empirical Potential Energy Functions. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5169-5177.	3.1	30
18	Advanced Monte Carlo Approach To Study Evolution of Quartz Surface during the Dissolution Process. <i>Journal of the American Chemical Society</i> , 2009, 131, 9538-9546.	13.7	30

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19	Modeling Diversity in Structures of Bacterial Outer Membrane Lipids. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 811-824.	5.3	30
20	Palmitoylation of Claudin-5 Proteins Influences Their Lipid Domain Affinity and Tight Junction Assembly at the Blood–Brain Barrier Interface. <i>Journal of Physical Chemistry B</i> , 2019, 123, 983-993.	2.6	27
21	The ghrelin O-acyltransferase structure reveals a catalytic channel for transmembrane hormone acylation. <i>Journal of Biological Chemistry</i> , 2019, 294, 14166-14174.	3.4	26
22	Combinatorial approaches to evaluate nanodiamond uptake and induced cellular fate. <i>Nanotechnology</i> , 2016, 27, 085107.	2.6	19
23	Computational Nanoscopy of Tight Junctions at the Blood–Brain Barrier Interface. <i>International Journal of Molecular Sciences</i> , 2019, 20, 5583.	4.1	18
24	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. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11643-11646.	2.5	17
25	Obtaining Protein Association Energy Landscape for Integral Membrane Proteins. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6444-6455.	5.3	17
26	Optical Signature of Formation of Protein Corona in the Firefly Luciferase-CdSe Quantum Dot Complex. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5224-5228.	5.3	16
27	A Structure–Property Relationship Study of the Well-Defined Telodendrimers to Improve Hemocompatibility of Nanocarriers for Anticancer Drug Delivery. <i>Langmuir</i> , 2014, 30, 6878-6888.	3.5	16
28	Molecular mechanism of ultrasound interaction with a blood brain barrier model. <i>Journal of Chemical Physics</i> , 2020, 153, 045104.	3.0	15
29	Theoretical advances in the dissolution studies of mineral–water interfaces. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 271-284.	1.4	13
30	Role of Intrasurface Hydrogen Bonding on Silica Dissolution. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2267-2272.	3.1	13
31	Drug-Specific Design of Telodendrimer Architecture for Effective Doxorubicin Encapsulation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9766-9777.	2.6	13
32	Dynamics of OmpF Trimer Formation in the Bacterial Outer Membrane of <i>Escherichia coli</i> . <i>Langmuir</i> , 2018, 34, 5623-5634.	3.5	13
33	Non-canonical lipoproteins with programmable assembly and architecture. <i>Chemical Communications</i> , 2020, 56, 10281-10284.	4.1	12
34	Paracellular Gatekeeping: What Does It Take for an Ion to Pass Through a Tight Junction Pore?. <i>Langmuir</i> , 2020, 36, 6757-6764.	3.5	10
35	Persister control by leveraging dormancy associated reduction of antibiotic efflux. <i>PLoS Pathogens</i> , 2021, 17, e1010144.	4.7	10
36	Development of effective stochastic potential method using random matrix theory for efficient conformational sampling of semiconductor nanoparticles at non-zero temperatures. <i>Journal of Chemical Physics</i> , 2018, 149, 014103.	3.0	7

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37	Interaction of amphiphilic coumarin with DPPC/DPPS lipid bilayer: effects of concentration and alkyl tail length. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15197-15207.	2.8	7
38	Predicting selectivity of paracellular pores for biomimetic applications. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 686-696.	3.4	7
39	Development of the computational antibiotic screening platform (CLASP) to aid in the discovery of new antibiotics. <i>Soft Matter</i> , 2021, 17, 2725-2736.	2.7	6
40	Signaling Factor Interactions with Polysaccharide Aggregates of Bacterial Biofilms. <i>Langmuir</i> , 2015, 31, 1958-1966.	3.5	4
41	Adaptive Recombinant Nanoworms from Genetically Encodable Star Amphiphiles. <i>Biomacromolecules</i> , 2022, 23, 863-876.	5.4	4
42	Salt Destabilization of Cationic Colistin Complexation within Polyanionic Microgels. <i>Macromolecules</i> , 2022, 55, 1736-1746.	4.8	4
43	High-Level Antibiotic Tolerance of a Clinically Isolated <i>Enterococcus faecalis</i> Strain. <i>Applied and Environmental Microbiology</i> , 2020, 87, .	3.1	2
44	Rational identification and characterisation of peptide ligands for targeting polysialic acid. <i>Scientific Reports</i> , 2020, 10, 7697.	3.3	1
45	Probing Mechanisms of Bacterial Infection through Molecular Dynamics Simulations. , 2013, , .		0