

Beena Rai

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

67
papers

1,577
citations

22
h-index

38
g-index

71
ext. papers

1,916
ext. citations

4
avg, IF

5.53
L-index

#	Paper	IF	Citations
67	Capturing the synergistic effects between corrosion inhibitor molecules using density functional theory and ReaxFF simulations - A case for benzyl azide and butyn-1-ol on Cu surface. <i>Corrosion Science</i> , 2022 , 195, 109960	6.8	3
66	Development of kinetic models for prediction of reducing sugar content in potatoes using literature data on multiple potato varieties. <i>LWT - Food Science and Technology</i> , 2022 , 155, 112986	5.4	1
65	A machine learning framework for urban mining: A case study on recovery of copper from printed circuit boards. <i>Minerals Engineering</i> , 2022 , 180, 107479	4.9	1
64	Coronavirus: a comparative analysis of detection technologies in the wake of emerging variants.. <i>Infection</i> , 2022 , 1	5.8	3
63	Temperature and humidity based models for the prediction of transpiration rate in potatoes during storage. <i>Journal of Food Process Engineering</i> , 2021 , 44, e13626	2.4	3
62	Effect of Temperature and Salt Concentration on the Properties of Electrolyte for Sodium-Ion Batteries. <i>Springer Proceedings in Energy</i> , 2021 , 1071-1081	0.2	
61	Recovery of Neodymium and Dysprosium from Waste Hard Disk Magnets: Roasting, Selective Leaching, Extraction and Stripping. <i>Transactions of the Indian Institute of Metals</i> , 2021 , 74, 1855-1863	1.2	1
60	AI-based soft-sensor for shelf life prediction of Kesar Mango. <i>SN Applied Sciences</i> , 2021 , 3, 1	1.8	1
59	Effect of temperature on concentrated electrolytes for advanced lithium ion batteries. <i>Journal of Chemical Physics</i> , 2021 , 154, 214503	3.9	2
58	In-silico screening of database for finding potential sweet molecules: A combined data and structure based modeling approach. <i>Food Chemistry</i> , 2021 , 343, 128538	8.5	6
57	A Deep Learning-Based Fruit Quality Assessment System 2021 , 187-192		
56	design of peptides with binding to the receptor binding domain (RBD) of the SARS-CoV-2 and their utility in bio-sensor development for SARS-CoV-2 detection.. <i>RSC Advances</i> , 2021 , 11, 3816-3826	3.7	8
55	Integrated Generate, Make, and Test For Formulated Products using Knowledge Graphs. <i>Data Intelligence</i> , 2021 , 3, 340-375	3	1
54	Solvation shell dynamics explains charge transport characteristics of LIB electrolytes. <i>Journal of Molecular Liquids</i> , 2021 , 338, 116613	6	2
53	Multiscale Modeling of Skin Electroporation. <i>Langmuir</i> , 2020 , 36, 6651-6660	4	1
52	Imidazole derivatives as corrosion inhibitors for copper: A DFT and reactive force field study. <i>Corrosion Science</i> , 2020 , 171, 108724	6.8	28
51	Molecular mechanism of the skin permeation enhancing effect of ethanol: a molecular dynamics study.. <i>RSC Advances</i> , 2020 , 10, 12234-12248	3.7	13

50	Development and application of coarse-grained MARTINI model of skin lipid ceramide [AP]. <i>Journal of Molecular Modeling</i> , 2020 , 26, 182	2	1
49	Permeation of nanoparticles across the intestinal lipid membrane: dependence on shape and surface chemistry studied through molecular simulations. <i>Nanoscale</i> , 2020 , 12, 6318-6333	7.7	25
48	Interfacial structure in the liquid-liquid extraction of rare earth elements by phosphoric acid ligands: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 4177-4192	3.6	5
47	Amino acids as copper corrosion inhibitors: A density functional theory approach. <i>Applied Surface Science</i> , 2020 , 514, 145905	6.7	52
46	Generate and Test for Formulated Product Variants With Information Extraction and an In-Silico Model. <i>Advances in E-Business Research Series</i> , 2020 , 223-250	0.4	2
45	Molecular dynamics investigation of electric field altered behavior of lithium ion battery electrolytes. <i>Journal of Molecular Liquids</i> , 2020 , 300, 112252	6	16
44	Applied machine learning for predicting the lanthanide-ligand binding affinities. <i>Scientific Reports</i> , 2020 , 10, 14322	4.9	5
43	An inherent instability study using ab initio computational methods and experimental validation of Pb(SCN) based perovskites for solar cell applications. <i>Scientific Reports</i> , 2020 , 10, 15241	4.9	4
42	Computer-Aided Design of Nanoparticles for Transdermal Drug Delivery. <i>Methods in Molecular Biology</i> , 2020 , 2059, 225-237	1.4	2
41	Materials Design in Digital Era: Challenges and Opportunities. <i>Transactions of the Indian Institute of Metals</i> , 2019 , 72, 2199-2208	1.2	0
40	Structural and barrier properties of the skin ceramide lipid bilayer: a molecular dynamics simulation study. <i>Journal of Molecular Modeling</i> , 2019 , 25, 140	2	7
39	Effect of Chemical Permeation Enhancers on Skin Permeability: In silico screening using Molecular Dynamics simulations. <i>Scientific Reports</i> , 2019 , 9, 1456	4.9	51
38	Bulk and surface DFT investigations of inorganic halide perovskites screened using machine learning and materials property databases. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 19423-19436	3.6	29
37	Multiscale analysis of large-strain deformation behaviour of random cross-linked elastomers. <i>Molecular Simulation</i> , 2019 , 45, 111-119	2	2
36	Molecular dynamics study of propylene carbonate based concentrated electrolyte solutions for lithium ion batteries. <i>Journal of Molecular Liquids</i> , 2019 , 278, 97-104	6	11
35	In-silico prediction of sweetness using structure-activity relationship models. <i>Food Chemistry</i> , 2018 , 253, 127-131	8.5	17
34	In-silico design of nanoparticles for transdermal drug delivery application. <i>Nanoscale</i> , 2018 , 10, 4940-4951	7	31
33	Electroporation of Skin Stratum Corneum Lipid Bilayer and Molecular Mechanism of Drug Transport: A Molecular Dynamics Study. <i>Langmuir</i> , 2018 , 34, 5860-5870	4	19

32	Effect of Salt Concentration on Properties of Lithium Ion Battery Electrolytes: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 8173-8181	3.8	47
31	Can carboxymethyl cellulose be used as a selective flocculant for beneficiating alumina-rich iron ore slimes? A density functional theory and experimental study. <i>Minerals Engineering</i> , 2018 , 121, 47-54	4.9	18
30	Molecular mechanism of transdermal co-delivery of interferon-alpha protein with gold nanoparticle via molecular dynamics study. <i>Molecular Simulation</i> , 2018 , 44, 274-284	2	8
29	Unravelling the mechanisms of corrosion inhibition of iron by henna extract: A density functional theory study. <i>Corrosion Science</i> , 2018 , 142, 102-109	6.8	35
28	Differential Stabilization of the Metal-Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 17209-17217	3.9	4
27	Effect of surface coverage and chemistry on self-assembly of monolayer protected gold nanoparticles: a molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25883-25891	3.6	19
26	Impact of the ceramide subspecies on the nanostructure of stratum corneum lipids using neutron scattering and molecular dynamics simulations. Part I: impact of CER[NS]. <i>Chemistry and Physics of Lipids</i> , 2018 , 214, 58-68	3.7	14
25	Modeling self-assembly of surfactants at interfaces. <i>Current Opinion in Chemical Engineering</i> , 2017 , 15, 84-94	5.4	8
24	Molecular dynamics simulation study of translocation of fullerene C through skin bilayer: effect of concentration on barrier properties. <i>Nanoscale</i> , 2017 , 9, 4114-4127	7.7	39
23	Transdermal cellular membrane penetration of proteins with gold nanoparticles: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 7537-7545	3.6	33
22	Guar gum as a selective flocculant for the beneficiation of alumina rich iron ore slimes: Density functional theory and experimental studies. <i>Minerals Engineering</i> , 2017 , 109, 144-152	4.9	20
21	Effect of Size and Surface Charge of Gold Nanoparticles on their Skin Permeability: A Molecular Dynamics Study. <i>Scientific Reports</i> , 2017 , 7, 45292	4.9	105
20	In-Silico Skin Model: A Multiscale Simulation Study of Drug Transport. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 2027-2034	6.1	22
19	Selective Flocculation of Iron Ore Slimes: Results of Successful Pilot Plant Trials at Tata Steel, Noamundi. <i>Transactions of the Indian Institute of Metals</i> , 2017 , 70, 411-419	1.2	16
18	Molecular Dynamics Simulation Study of Permeation of Molecules through Skin Lipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8987-96	3.4	64
17	Molecular Dynamics Simulation of Skin Lipids: Effect of Ceramide Chain Lengths on Bilayer Properties. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 12536-12546	3.4	37
16	Penetration of Gold Nanoparticles through Human Skin: Unraveling Its Mechanisms at the Molecular Scale. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 7133-42	3.4	50
15	Concurrent reconciliation of chemical and mineral assays for mineral processing circuits. <i>International Journal of Mineral Processing</i> , 2016 , 146, 1-9		7

14	Density Functional Theory Computations for Design of Salicylaldoxime Derivatives as Selective Reagents in Solvent Extraction of Copper. <i>Transactions of the Indian Institute of Metals</i> , 2016 , 69, 135-141 ^{1,2}	1.2	11
13	Quantitative Estimation of Mineral Phases from Chemical Assays and Powder X-Ray Diffraction Rietveld Analysis: A Case Study on Selective Flocculation of Iron Ore Slimes. <i>Transactions of the Indian Institute of Metals</i> , 2016 , 69, 125-133	1.2	3
12	Molecular Dynamics Simulation Study of Skin Lipids: Effects of the Molar Ratio of Individual Components over a Wide Temperature Range. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11643-55	3-4	49
11	Stable Nanofluids for Convective Heat Transfer Applications. <i>Journal of Heat Transfer</i> , 2014 , 136, 021704.8	4.8	8
10	Processing of Alumina-Rich Iron Ore Slimes: Is the Selective Dispersion Flocculation Flotation the Solution We Are Looking for the Challenging Problem Facing the Indian Iron and Steel Industry?. <i>Transactions of the Indian Institute of Metals</i> , 2013 , 66, 447-456	1.2	22
9	A molecular dynamics study of the interaction of oleate and dodecylammonium chloride surfactants with complex aluminosilicate minerals. <i>Journal of Colloid and Interface Science</i> , 2011 , 362, 510-6	9-3	143
8	Design of highly selective industrial performance chemicals: a molecular modelling approach. <i>Molecular Simulation</i> , 2008 , 34, 1209-1214	2	33
7	Rational Design of Dispersants by Molecular Modeling for Advanced Ceramics Processing Applications. <i>KONA Powder and Particle Journal</i> , 2004 , 22, 151-158	3-4	16
6	Molecular dynamic simulations of self-assembled alkylthiolate monolayers on an Au(III) surface. <i>Langmuir</i> , 2004 , 20, 3138-44	4	78
5	Molecular modeling and rational design of flotation reagents. <i>International Journal of Mineral Processing</i> , 2003 , 72, 95-110		73
4	Molecular Modeling of Interactions of Alkyl Hydroxamates with Calcium Minerals. <i>Journal of Colloid and Interface Science</i> , 2002 , 256, 106-113	9-3	87
3	Design of tailor-made surfactants for industrial applications using a molecular modelling approach. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2002 , 205, 139-148	5-1	53
2	Molecular Modeling of Interactions of Diphosphonic Acid Based Surfactants with Calcium Minerals. <i>Langmuir</i> , 2002 , 18, 932-940	4	101
1	Analyzing the physical and biochemical changes in strawberries during storage at different temperatures and the development of kinetic models. <i>Journal of Food Measurement and Characterization</i> , 2011 , 1	2.8	0