Beena Rai

List of Publications by Citations

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	A molecular dynamics study of the interaction of oleate and dodecylammonium chloride surfactants with complex aluminosilicate minerals. *Journal of Colloid and Interface Science*, **2011**, 362, 510-6	9.3	143
66	Effect of Size and Surface Charge of Gold Nanoparticles on their Skin Permeability: A Molecular Dynamics Study. *Scientific Reports*, **2017**, 7, 45292	4.9	105
65	Molecular Modeling of Interactions of Diphosphonic Acid Based Surfactants with Calcium Minerals. *Langmuir*, **2002**, 18, 932-940	4	101
64	Molecular Modeling of Interactions of Alkyl Hydroxamates with Calcium Minerals. *Journal of Colloid and Interface Science*, **2002**, 256, 106-113	9.3	87
63	Molecular dynamic simulations of self-assembled alkylthiolate monolayers on an Au(III) surface. *Langmuir*, **2004**, 20, 3138-44	4	78
62	Molecular modeling and rational design of flotation reagents. *International Journal of Mineral Processing*, **2003**, 72, 95-110		73
61	Molecular Dynamics Simulation Study of Permeation of Molecules through Skin Lipid Bilayer. *Journal of Physical Chemistry B*, **2016**, 120, 8987-96	3.4	64
60	Design of tailor-made surfactants for industrial applications using a molecular modelling approach. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2002**, 205, 139-148	5.1	53
59	Amino acids as copper corrosion inhibitors: A density functional theory approach. *Applied Surface Science*, **2020**, 514, 145905	6.7	52
58	Effect of Chemical Permeation Enhancers on Skin Permeability: In silico screening using Molecular Dynamics simulations. *Scientific Reports*, **2019**, 9, 1456	4.9	51
57	Penetration of Gold Nanoparticles through Human Skin: Unraveling Its Mechanisms at the Molecular Scale. *Journal of Physical Chemistry B*, **2016**, 120, 7133-42	3.4	50
56	Molecular Dynamics Simulation Study of Skin Lipids: Effects of the Molar Ratio of Individual Components over a Wide Temperature Range. *Journal of Physical Chemistry B*, **2015**, 119, 11643-55	3.4	49
55	Effect of Salt Concentration on Properties of Lithium Ion Battery Electrolytes: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2018**, 122, 8173-8181	3.8	47
54	Molecular dynamics simulation study of translocation of fullerene C through skin bilayer: effect of concentration on barrier properties. *Nanoscale*, **2017**, 9, 4114-4127	7.7	39
53	Molecular Dynamics Simulation of Skin Lipids: Effect of Ceramide Chain Lengths on Bilayer Properties. *Journal of Physical Chemistry B*, **2016**, 120, 12536-12546	3.4	37
52	Unravelling the mechanisms of corrosion inhibition of iron by henna extract: A density functional theory study. *Corrosion Science*, **2018**, 142, 102-109	6.8	35
51	Transdermal cellular membrane penetration of proteins with gold nanoparticles: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2017**, 19, 7537-7545	3.6	33

50	Design of highly selective industrial performance chemicals: a molecular modelling approach. *Molecular Simulation*, **2008**, 34, 1209-1214	2	33
49	In-silico design of nanoparticles for transdermal drug delivery application. *Nanoscale*, **2018**, 10, 4940-4951	7.7	31
48	Bulk and surface DFT investigations of inorganic halide perovskites screened using machine learning and materials property databases. *Physical Chemistry Chemical Physics*, **2019**, 21, 19423-19436	3.6	29
47	Imidazole derivatives as corrosion inhibitors for copper: A DFT and reactive force field study. *Corrosion Science*, **2020**, 171, 108724	6.8	28
46	Permeation of nanoparticles across the intestinal lipid membrane: dependence on shape and surface chemistry studied through molecular simulations. *Nanoscale*, **2020**, 12, 6318-6333	7.7	25
45	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?. *Transactions of the Indian Institute of Metals*, **2013**, 66, 447-456	1.2	22
44	In-Silico Skin Model: A Multiscale Simulation Study of Drug Transport. *Journal of Chemical Information and Modeling*, **2017**, 57, 2027-2034	6.1	22
43	Guar gum as a selective flocculant for the beneficiation of alumina rich iron ore slimes: Density functional theory and experimental studies. *Minerals Engineering*, **2017**, 109, 144-152	4.9	20
42	Electroporation of Skin Stratum Corneum Lipid Bilayer and Molecular Mechanism of Drug Transport: A Molecular Dynamics Study. *Langmuir*, **2018**, 34, 5860-5870	4	19
41	Effect of surface coverage and chemistry on self-assembly of monolayer protected gold nanoparticles: a molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2018**, 20, 25883-25891	3.6	19
40	Can carboxymethyl cellulose be used as a selective flocculant for beneficiating alumina-rich iron ore slimes? A density functional theory and experimental study. *Minerals Engineering*, **2018**, 121, 47-54	4.9	18
39	In-silico prediction of sweetness using structure-activity relationship models. *Food Chemistry*, **2018**, 253, 127-131	8.5	17
38	Selective Flocculation of Iron Ore Slimes: Results of Successful Pilot Plant Trials at Tata Steel, Noamundi. *Transactions of the Indian Institute of Metals*, **2017**, 70, 411-419	1.2	16
37	Rational Design of Dispersants by Molecular Modeling for Advanced Ceramics Processing Applications. *KONA Powder and Particle Journal*, **2004**, 22, 151-158	3.4	16
36	Molecular dynamics investigation of electric field altered behavior of lithium ion battery electrolytes. *Journal of Molecular Liquids*, **2020**, 300, 112252	6	16
35	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]. *Chemistry and Physics of Lipids*, **2018**, 214, 58-68	3.7	14
34	Molecular mechanism of the skin permeation enhancing effect of ethanol: a molecular dynamics study.. *RSC Advances*, **2020**, 10, 12234-12248	3.7	13
33	Density Functional Theory Computations for Design of Salicylaldoxime Derivatives as Selective Reagents in Solvent Extraction of Copper. *Transactions of the Indian Institute of Metals*, **2016**, 69, 135-141	1.2	11

32	Molecular dynamics study of propylene carbonate based concentrated electrolyte solutions for lithium ion batteries. *Journal of Molecular Liquids*, **2019**, 278, 97-104	6	11
31	Modeling self-assembly of surfactants at interfaces. *Current Opinion in Chemical Engineering*, **2017**, 15, 84-94	5.4	8
30	Molecular mechanism of transdermal co-delivery of interferon-alpha protein with gold nanoparticle – a molecular dynamics study. *Molecular Simulation*, **2018**, 44, 274-284	2	8
29	Stable Nanofluids for Convective Heat Transfer Applications. *Journal of Heat Transfer*, **2014**, 136, 021704	1.8	8
28	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.. *RSC Advances*, **2021**, 11, 3816-3826	3.7	8
27	Structural and barrier properties of the skin ceramide lipid bilayer: a molecular dynamics simulation study. *Journal of Molecular Modeling*, **2019**, 25, 140	2	7
26	Concurrent reconciliation of chemical and mineral assays for mineral processing circuits. *International Journal of Mineral Processing*, **2016**, 146, 1-9		7
25	In-silico screening of database for finding potential sweet molecules: A combined data and structure based modeling approach. *Food Chemistry*, **2021**, 343, 128538	8.5	6
24	Interfacial structure in the liquid-liquid extraction of rare earth elements by phosphoric acid ligands: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2020**, 22, 4177-4192	3.6	5
23	Applied machine learning for predicting the lanthanide-ligand binding affinities. *Scientific Reports*, **2020**, 10, 14322	4.9	5
22	An inherent instability study using ab initio computational methods and experimental validation of Pb(SCN) based perovskites for solar cell applications. *Scientific Reports*, **2020**, 10, 15241	4.9	4
21	Differential Stabilization of the Metal–Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. *Industrial & Engineering Chemistry Research*, **2018**, 57, 17209-17217	3.9	4
20	Temperature and humidity based models for the prediction of transpiration rate in potatoes during storage. *Journal of Food Process Engineering*, **2021**, 44, e13626	2.4	3
19	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. *Corrosion Science*, **2022**, 195, 109960	6.8	3
18	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. *Transactions of the Indian Institute of Metals*, **2016**, 69, 125-133	1.2	3
17	Coronavirus: a comparative analysis of detection technologies in the wake of emerging variants.. *Infection*, **2022**, 1	5.8	3
16	Generate and Test for Formulated Product Variants With Information Extraction and an In-Silico Model. *Advances in E-Business Research Series*, **2020**, 223-250	0.4	2
15	Effect of temperature on concentrated electrolytes for advanced lithium ion batteries. *Journal of Chemical Physics*, **2021**, 154, 214503	3.9	2

List of Publications

14	Multiscale analysis of large-strain deformation behaviour of random cross-linked elastomers. *Molecular Simulation*, **2019**, 45, 111-119	2	2
13	Computer-Aided Design of Nanoparticles for Transdermal Drug Delivery. *Methods in Molecular Biology*, **2020**, 2059, 225-237	1.4	2
12	Solvation shell dynamics explains charge transport characteristics of LIB electrolytes. *Journal of Molecular Liquids*, **2021**, 338, 116613	6	2
11	Multiscale Modeling of Skin Electroporation. *Langmuir*, **2020**, 36, 6651-6660	4	1
10	Development and application of coarse-grained MARTINI model of skin lipid ceramide [AP]. *Journal of Molecular Modeling*, **2020**, 26, 182	2	1
9	Development of kinetic models for prediction of reducing sugar content in potatoes using literature data on multiple potato varieties. *LWT - Food Science and Technology*, **2022**, 155, 112986	5.4	1
8	Recovery of Neodymium and Dysprosium from Waste Hard Disk Magnets: Roasting, Selective Leaching, Extraction and Stripping. *Transactions of the Indian Institute of Metals*, **2021**, 74, 1855-1863	1.2	1
7	AI-based soft-sensor for shelf life prediction of Kesar mango. *SN Applied Sciences*, **2021**, 3, 1	1.8	1
6	Integrated Generate, Make, and Test for Formulated Products using Knowledge Graphs. *Data Intelligence*, **2021**, 3, 340-375	3	1
5	A machine learning framework for urban mining: A case study on recovery of copper from printed circuit boards. *Minerals Engineering*, **2022**, 180, 107479	4.9	1
4	Materials Design in Digital Era: Challenges and Opportunities. *Transactions of the Indian Institute of Metals*, **2019**, 72, 2199-2208	1.2	0
3	Analyzing the physical and biochemical changes in strawberries during storage at different temperatures and the development of kinetic models. *Journal of Food Measurement and Characterization*,1	2.8	0
2	Effect of Temperature and Salt Concentration on the Properties of Electrolyte for Sodium-Ion Batteries. *Springer Proceedings in Energy*, **2021**, 1071-1081	0.2	
1	A Deep Learning-Based Fruit Quality Assessment System **2021**, 187-192		