Neeraj Rai

List of Publications by Year in descending order

46 papers	1,684 citations	304743 22 h-index	289244 40 g-index
46 all docs	46 docs citations	46 times ranked	1961 citing authors

#	Article	IF	Citations
1	Insights into Sorption and Molecular Transport of Aqueous Glucose into Zeolite Nanopores. Journal of Physical Chemistry B, 2022, 126, 1352-1364.	2.6	1
2	Benzobisthiadiazole-based high-spin donorâ€“acceptor conjugated polymers with localized spin distribution. Materials Advances, 2021, 2, 2943-2955.	5.4	10
3	Effect of water models on structure and dynamics of lignin in solution. AIP Advances, 2021, 11, .	1.3	10
4	Probing Interfacial Halogen-Bonding Effects with Halogenated Organic Dyes and a Lewis Base-Decorated Transition Metal-Based Redox Shuttle at a Metal Oxide Interface in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2021, 125, 17647-17659.	3.1	13
5	Evolution of the electronic structure in open-shell donor-acceptor organic semiconductors. Nature Communications, 2021, 12, 5889.	12.8	47
6	Donor-Acceptor Conjugated Macrocycles with Polyradical Character and Global Aromaticity. IScience, 2020, 23, 101675.	4.1	8
7	Open-shell donorâ€“Ï€â€“acceptor conjugated metal-free dyes for dye-sensitized solar cells. Molecular Systems Design and Engineering, 2020, 5, 1477-1490.	3.4	9
8	Bimetallic Ruâ€“Mo Phosphide Catalysts for the Hydrogenation of CO₂ to Methanol. Industrial & Engineering Chemistry Research, 2020, 59, 6931-6943.	3.7	24
9	Hydrogenation of cinnamaldehyde to cinnamyl alcohol with metal phosphides: Catalytic consequences of product and pyridine doping. Applied Catalysis B: Environmental, 2020, 277, 119272.	20.2	33
10	Probing Early-Stage Aggregation of Low Molecular Weight Gelator in an Organic Solvent. Journal of Physical Chemistry B, 2020, 124, 2277-2288.	2.6	7
11	CO2 sorption in triethyl(butyl)phosphonium 2-cyanopyrrolide ionic liquid via first principles simulations. Journal of Molecular Liquids, 2019, 292, 111323.	4.9	7
12	Wide Potential Window Supercapacitors Using Openâ€Shell Donorâ€“Acceptor Conjugated Polymers with Stable Nâ€Doped States. Advanced Energy Materials, 2019, 9, 1902806.	19.5	53
13	Solvation effect on binding modes of model lignin dimer compounds on MWW 2D-zeolite. Journal of Chemical Physics, 2019, 151, 114708.	3.0	2
14	Optimization of microbial cell disruption using pressurized CO2 for improving lipid recovery from wet biomass. Bioprocess and Biosystems Engineering, 2019, 42, 763-776.	3.4	5
15	A high-spin ground-state donor-acceptor conjugated polymer. Science Advances, 2019, 5, eaav2336.	10.3	72
16	Direct synthesis of furfuryl alcohol from furfural: catalytic performance of monometallic and bimetallic Mo and Ru phosphides. Catalysis Science and Technology, 2019, 9, 3656-3668.	4.1	35
17	Molecular insights into ionic liquid/aqueous interface of phosphonium based phase-separable ionic liquids. AIP Advances, 2019, 9, 045115.	1.3	10
18	Transferable Potentials for Chloroethenes: Insights into Nonideal Solution Behavior of Environmental Contaminants. ACS Omega, 2018, 3, 3646-3654.	3.5	3

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19	Solubility of CO2 in triglycerides using Monte Carlo simulations. Fluid Phase Equilibria, 2018, 476, 39-47.	2.5	10
20	Performance of density functionals for modeling vapor liquid equilibria of CO₂ and SO₂. Journal of Computational Chemistry, 2018, 39, 397-406.	3.3	12
21	A molecular dynamics investigation of actinylâ€“ligand speciation in aqueous solution. Physical Chemistry Chemical Physics, 2018, 20, 15753-15763.	2.8	13
22	Improving the lipid recovery from wet oleaginous microorganisms using different pretreatment techniques. Bioresource Technology, 2018, 267, 743-755.	9.6	22
23	Mechanistic insights into hydrodeoxygenation of phenol on bimetallic phosphide catalysts. Catalysis Science and Technology, 2018, 8, 4083-4096.	4.1	31
24	Iodine binding with thiophene and furan based dyes for DSCs. Physical Chemistry Chemical Physics, 2018, 20, 17859-17870.	2.8	15
25	Predicting vapor liquid equilibria using density functional theory: A case study of argon. Journal of Chemical Physics, 2018, 148, 224501.	3.0	10
26	Cassandra: An open source Monte Carlo package for molecular simulation. Journal of Computational Chemistry, 2017, 38, 1727-1739.	3.3	106
27	Molecular Insights into Gelation of Di-Fmoc-<scp>l</scp>-Lysine in Organic Solventâ€“Water Mixtures. ACS Omega, 2017, 2, 1864-1874.	3.5	30
28	Microbial cell disruption for improving lipid recovery using pressurized CO2: Role of CO2solubility in cell suspension, sugar broth, and spent media. Biotechnology Progress, 2017, 33, 737-748.	2.6	21
29	Composition-directed Fe_XMo_{2â^'X}P bimetallic catalysts for hydrodeoxygenation reactions. Catalysis Science and Technology, 2017, 7, 1857-1867.	4.1	48
30	Measurement and correlation of solubility of carbon dioxide in triglycerides. Journal of Chemical Thermodynamics, 2017, 104, 252-260.	2.0	14
31	Phase Equilibria and Condensed Phase Properties of Fluorinated Alkanes via First Principles Simulations. ChemistrySelect, 2017, 2, 11969-11976.	1.5	4
32	Vapor Liquid Equilibria of Hydrofluorocarbons Using Dispersion-Corrected and Nonlocal Density Functionals. Journal of Chemical Theory and Computation, 2016, 12, 3295-3304.	5.3	11
33	Dynamics of actinyl ions in water: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2014, 16, 8060-8069.	2.8	33
34	Development and application of effective pairwise potentials for UO2n+, NpO2n+, PuO2n+, and AmO2n+ (n = 1, 2) ions with water. Physical Chemistry Chemical Physics, 2013, 15, 15954.	2.8	42
35	Role of Silanol Group in Sn-Beta Zeolite for Glucose Isomerization and Epimerization Reactions. ACS Catalysis, 2013, 3, 2294-2298.	11.2	128
36	Transferable Potentials for Phase Equilibria. 10. Explicit-Hydrogen Description of Substituted Benzenes and Polycyclic Aromatic Compounds. Journal of Physical Chemistry B, 2013, 117, 273-288.	2.6	95

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37	Force Field Development for Actinyl Ions via Quantum Mechanical Calculations: An Approach to Account for Many Body Solvation Effects. Journal of Physical Chemistry B, 2012, 116, 10885-10897.	2.6	38
38	Critical behaviour and vapour-liquid coexistence of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquidsvia Monte Carlo simulations. Faraday Discussions, 2012, 154, 53-69.	3.2	59
39	Vaporâ€“Liquid Coexistence and Critical Behavior of Ionic Liquids via Molecular Simulations. Journal of Physical Chemistry Letters, 2011, 2, 1439-1443.	4.6	71
40	Monte Carlo simulations of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB): Pressure and temperature effects for the solid phase and vapor-liquid phase equilibria. Journal of Chemical Physics, 2008, 129, 194510.	3.0	37
41	Application of the TraPPE Force Field for Predicting the Hildebrand Solubility Parameters of Organic Solvents and Monomer Units. Journal of Chemical Theory and Computation, 2008, 4, 136-144.	5.3	32
42	Transferable Potentials for Phase Equilibria. 9. Explicit Hydrogen Description of Benzene and Five-Membered and Six-Membered Heterocyclic Aromatic Compounds. Journal of Physical Chemistry B, 2007, 111, 10790-10799.	2.6	185
43	Pressure Dependence of the Hildebrand Solubility Parameter and the Internal Pressure:â€‰ Monte Carlo Simulations for External Pressures up to 300 MPa. Journal of Physical Chemistry C, 2007, 111, 15634-15641.	3.1	44
44	Prediction of the bubble point pressure for the binary mixture of ethanol and 1,1,1,2,3,3,3-heptafluoropropane from Gibbs ensemble Monte Carlo simulations using the TraPPE force field. Fluid Phase Equilibria, 2007, 260, 199-211.	2.5	11
45	Transferable Potentials for Phase Equilibria. 7. Primary, Secondary, and Tertiary Amines, Nitroalkanes and Nitrobenzene, Nitriles, Amides, Pyridine, and Pyrimidine. Journal of Physical Chemistry B, 2005, 109, 18974-18982.	2.6	212
46	Designing Donor-Acceptor Conjugated Macrocycles with Polyradical Character and Global (Anti)Aromaticity. SSRN Electronic Journal, 0, , .	0.4	1