Vivek S Bharadwaj

List of Publications by Year
in descending order

28	542	623734	642732
papers	citations	14 h-index	23 g-index

32	32	32	809
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in Multiscale Modeling of Lignocellulosic Biomass. ACS Sustainable Chemistry and Engineering, 2020, 8, 3512-3531.	6.7	79
2	Structural, mutagenic and inÂsilico studies of xyloglucan fucosylation in Arabidopsis thaliana suggest a waterâ€mediated mechanism. Plant Journal, 2017, 91, 931-949.	5.7	53
3	Nanomechanics of cellulose deformation reveal molecular defects that facilitate natural deconstruction. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9825-9830.	7.1	40
4	Molecular Mechanism of Polysaccharide Acetylation by the Arabidopsis Xylan O-acetyltransferase XOAT1. Plant Cell, 2020, 32, 2367-2382.	6.6	32
5	Beyond the effectiveness factor: Multi-step reactions with intraparticle diffusion limitations. Chemical Engineering Journal, 2020, 380, 122507.	12.7	31
6	Insights into the Glycyl Radical Enzyme Active Site of Benzylsuccinate Synthase: A Computational Study. Journal of the American Chemical Society, 2013, 135, 12279-12288.	13.7	30
7	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. Wiley Interdisciplinary Reviews: Energy and Environment, 2018, 7, e297.	4.1	30
8	Impact of Water-Dilution on the Solvation Properties of the Ionic Liquid 1-Methyltriethoxy-3-ethylimidazolium Acetate for Model Biomass Molecules. Journal of Physical Chemistry B, 2017, 121, 843-853.	2.6	23
9	Understanding extreme fast charge limitations in carbonate mixtures. Journal of Materials Chemistry A, 2021, 9, 4858-4869.	10.3	21
10	Elucidating the conformational energetics of glucose and cellobiose in ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 10668-10678.	2.8	19
11	Locating Methyl-Etherified and Methyl-Esterified Uronic Acids in the Plant Cell Wall Pectic Polysaccharide Rhamnogalacturonan II. SLAS Technology, 2020, 25, 329-344.	1.9	19
12	In silico insights into the solvation characteristics of the ionic liquid 1-methyltriethoxy-3-ethylimidazolium acetate for cellulosic biomass. Physical Chemistry Chemical Physics, 2016, 18, 23715-23726.	2.8	17
13	Multi-scale simulation of reaction, transport and deactivation in a SBA-16 supported catalyst for the conversion of ethanol to butadiene. Catalysis Today, 2019, 338, 141-151.	4.4	17
14	The hydrolysis mechanism of a GH45 cellulase and its potential relation to lytic transglycosylase and expansin function. Journal of Biological Chemistry, 2020, 295, 4477-4487.	3.4	16
15	Acetylcholine Promotes Binding of Î±â€Conotoxin MII at Î±₃Î²₂ Nicotinic Acetylcholine Receptors. ChemBioChem, 2014, 15, 413-424.	2.6	14
16	Molecular Simulations of Fattyâ€Acid Methyl Esters and Representative Biodiesel Mixtures. ChemPhysChem, 2015, 16, 2810-2817.	2.1	14
17	Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism â€“ a gas-phaseab initiostudy. Physical Chemistry Chemical Physics, 2015, 17, 4054-4066.	2.8	14
18	Impact of water dilution and cation tail length on ionic liquid characteristics: Interplay between polar and non-polar interactions. Journal of Chemical Physics, 2016, 145, 064504.	3.0	14

#	Article	IF	Citations
19	Selective One-Dimensional ¹³Câ€“¹³C Spin-Diffusion Solid-State Nuclear Magnetic Resonance Methods to Probe Spatial Arrangements in Biopolymers Including Plant Cell Walls, Peptides, and Spider Silk. Journal of Physical Chemistry B, 2020, 124, 9870-9883.	2.6	11
20	Ex situ upgrading of pyrolysis vapors over PtTiO₂: extraction of apparent kinetics via hierarchical transport modeling. Reaction Chemistry and Engineering, 2021, 6, 125-137.	3.7	11
21	Different Behaviors of a Substrate in P450 Decarboxylase and Hydroxylase Reveal Reactivity-Enabling Actors. Scientific Reports, 2018, 8, 12826.	3.3	9
22	A site-differentiated [4Feâ€“4S] cluster controls electron transfer reactivity of Clostridium acetobutylicum [FeFe]-hydrogenase I. Chemical Science, 2022, 13, 4581-4588.	7.4	8
23	The impact of active site protonation on substrate ring conformation in Melanocarpus albomyces cellobiohydrolase Cel7B. Physical Chemistry Chemical Physics, 2015, 17, 16947-16958.	2.8	5
24	Mechanism and Reaction Energy Landscape for Apiose Cross-Linking by Boric Acid in Rhamnogalacturonan II. Journal of Physical Chemistry B, 2020, 124, 10117-10125.	2.6	5
25	Mass Transport Limitations and Kinetic Consequences of Corn Stover Deacetylation. Frontiers in Energy Research, 2022, 10, .	2.3	5
26	Rational enzyme design for controlled functionalization of acetylated xylan for cell-free polymer biosynthesis. Carbohydrate Polymers, 2021, 273, 118564.	10.2	4
27	Reply to Cosgrove: Non-enzymatic action of expansins. Journal of Biological Chemistry, 2020, 295, 6783.	3.4	0
28	Towards Elucidating Structureâ€“Spectra Relationships in Rhamnogalacturonan II: Computational Protocols for Accurate 13C and 1H Shifts for Apiose and Its Borate Esters. Frontiers in Molecular Biosciences, 2021, 8, 756219.	3.5	0