Arun Venkatnathan

List of Publications by Year
in descending order

28	668	840776 11	552781 26
papers	citations	h-index	g-index

29	29	29	730
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atomistic Simulations of Hydrated Nafion and Temperature Effects on Hydronium Ion Mobility. Journal of Physical Chemistry B, 2007, 111, 7234-7244.	2.6	212
2	Atomistic Simulation of Water Percolation and Proton Hopping in Nafion Fuel Cell Membrane. Journal of Physical Chemistry B, 2010, 114, 13681-13690.	2.6	125
3	Molecular dynamics simulations of side chain pendants of perfluorosulfonic acidpolymer electrolyte membranes. Journal of Materials Chemistry A, 2013, 1, 557-569.	10.3	37
4	Atomistic simulations of structure and dynamics of hydrated Aciplex polymer electrolyte membrane. Soft Matter, 2012, 8, 10827.	2.7	29
5	Interplay of Phase Separation, Tail Aggregation, and Micelle Formation in the Nanostructured Organization of Hydrated Imidazolium Ionic Liquid. Journal of Physical Chemistry B, 2014, 118, 8839-8847.	2.6	28
6	Molecular Simulations of Anion and Temperature Dependence on Structure and Dynamics of 1-Hexyl-3-methylimidazolium Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 14800-14806.	2.6	27
7	Quantum Chemistry Study of Proton Transport in Imidazole Chains. Journal of Physical Chemistry B, 2015, 119, 3213-3222.	2.6	24
8	Atomistic simulation study of the hydrated structure and transport dynamics of a novel multi acid side chain polyelectrolyte membrane. International Journal of Hydrogen Energy, 2017, 42, 27254-27268.	7.1	24
9	Mechanism of Proton Transport in Ionic-Liquid-Doped Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry B, 2013, 117, 14449-14456.	2.6	23
10	Molecular mechanism of CO₂ absorption in phosphonium amino acid ionic liquid. RSC Advances, 2016, 6, 55438-55443.	3.6	19
11	Nanostructure and Dynamics of Humidified Nafion/Graphene-Oxide Composites via Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 22864-22875.	3.1	16
12	Effect of Annealing on Structure and Diffusion in Hydrated Nafion Membranes. ACS Applied Polymer Materials, 2020, 2, 5058-5066.	4.4	13
13	Site-Specific Interactions in CO₂ Capture by Lysinate Anion and Role of Water Using Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 12647-12656.	3.1	12
14	Parametric dependence on shear viscosity of SPC/E water from equilibrium and non-equilibrium molecular dynamics simulations. Molecular Simulation, 2013, 39, 728-733.	2.0	11
15	A molecular investigation of the nanostructure and dynamics of phosphoricâ€“triflic acid blends of hydrated ABPBI [poly(2,5-benzimidazole)] polymer electrolyte membranes. Soft Matter, 2013, 9, 1122-1132.	2.7	9
16	Experimental and Theoretical Investigation of the Ion Conduction Mechanism of Tris(adiponitrile)perchloratosodium, a Self-Binding, Melt-Castable Crystalline Sodium Electrolyte. Chemistry of Materials, 2019, 31, 8850-8863.	6.7	9
17	Probing translational and rotational dynamics in hydrophilic/hydrophobic anion based imidazolium ionic liquidâ€“water mixtures. Soft Matter, 2018, 14, 6109-6118.	2.7	8
18	Quantum Mechanical Investigation of Proton Transport in Imidazolium Methanesulfonate Ionic liquid. Journal of Physical Chemistry C, 2017, 121, 7069-7080.	3.1	7

#	Article	IF	Citations
19	Computational investigation of a protic ionic liquid doped poly-benzimidazole fuel cell electrolyte. Journal of Molecular Liquids, 2020, 314, 113686.	4.9	7
20	Unravelling the structural and dynamical complexity of the equilibrium liquid grain-binding layer in highly conductive organic crystalline electrolytes. Journal of Materials Chemistry A, 2018, 6, 4394-4404.	10.3	6
21	Polymer chain length, phosphoric acid doping and temperature dependence on structure and dynamics of an ABPBI [poly(2,5-benzimidazole)] polymer electrolyte membrane. RSC Advances, 2014, 4, 19746-19755.	3.6	5
22	Effect of Concentration and Temperature on the Structure and Ion Transport in Diglyme-Based Sodium-Ion Electrolyte. Journal of Physical Chemistry B, 2022, 126, 2119-2129.	2.6	5
23	Solvate sponge crystals of (DMF)₃NaClO₄: reversible pressure/temperature controlled juicing in a melt/press-castable sodium-ion conductor. Chemical Science, 2021, 12, 5574-5581.	7.4	3
24	Mechanism of Ion Conduction and Dynamics in Tris(N,N-dimethylformamide) Perchloratosodium Solid Electrolytes. Journal of Physical Chemistry C, 2022, 126, 4744-4750.	3.1	3
25	Novel polyelectrolyte membranes for fuel and flow batteries: Insights from simulations. AIP Conference Proceedings, 2018, , .	0.4	2
26	Charge delocalization effects on Nafion structure and water /proton dynamics in hydrated environments. Fluid Phase Equilibria, 2020, 504, 112340.	2.5	1
27	Multiscale Modeling Examples: New Polyelectrolyte Nanocomposite Membranes for Perspective Fuel Cells and Flow Batteries. Springer Series in Materials Science, 2021, , 133-177.	0.6	1
28	Invoking chemical principles to predict the anions of dihydrooxazole family as prospective carbon capture moieties. Computational and Theoretical Chemistry, 2021, 1206, 113472.	2.5	0