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	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
2	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
3	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
4	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
5	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
6	Charge delocalization effects on Nafion structure and water /proton dynamics in hydrated environments. Fluid Phase Equilibria, 2020, 504, 112340.	2.5	1
7	Effect of Annealing on Structure and Diffusion in Hydrated Nafion Membranes. ACS Applied Polymer Materials, 2020, 2, 5058-5066.	4.4	13
8	Computational investigation of a protic ionic liquid doped poly-benzimidazole fuel cell electrolyte. Journal of Molecular Liquids, 2020, 314, 113686.	4.9	7
9	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
10	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
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	Probing translational and rotational dynamics in hydrophilic/hydrophobic anion based imidazolium ionic liquidâ€“water mixtures. Soft Matter, 2018, 14, 6109-6118.	2.7	8
13	Novel polyelectrolyte membranes for fuel and flow batteries: Insights from simulations. AIP Conference Proceedings, 2018, , .	0.4	2
14	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
15	Quantum Mechanical Investigation of Proton Transport in Imidazolium Methanesulfonate Ionic liquid. Journal of Physical Chemistry C, 2017, 121, 7069-7080.	3.1	7
16	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
17	Molecular mechanism of CO₂ absorption in phosphonium amino acid ionic liquid. RSC Advances, 2016, 6, 55438-55443.	3.6	19
18	Quantum Chemistry Study of Proton Transport in Imidazole Chains. Journal of Physical Chemistry B, 2015, 119, 3213-3222.	2.6	24

#	Article	IF	Citations
19	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
20	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
21	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
22	Molecular dynamics simulations of side chain pendants of perfluorosulfonic acidpolymer electrolyte membranes. Journal of Materials Chemistry A, 2013, 1, 557-569.	10.3	37
23	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
24	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
25	Mechanism of Proton Transport in Ionic-Liquid-Doped Perfluorosulfonic Acid Membranes. Journal of Physical Chemistry B, 2013, 117, 14449-14456.	2.6	23
26	Atomistic simulations of structure and dynamics of hydrated Aciplex polymer electrolyte membrane. Soft Matter, 2012, 8, 10827.	2.7	29
27	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
28	Atomistic Simulations of Hydrated Nafion and Temperature Effects on Hydronium Ion Mobility. Journal of Physical Chemistry B, 2007, 111, 7234-7244.	2.6	212