Nav Nidhi Rajput

List of Publications by Year
in descending order

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24 papers	2,191 citations	394421 19 h-index	642732 23 g-index
24 all docs	24 docs citations	24 times ranked	3272 citing authors

#	Article	IF	Citations
1	Non-encapsulation approach for high-performance Liâ€“S batteries through controlled nucleation and growth. Nature Energy, 2017, 2, 813-820.	39.5	326
2	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
3	The Coupling between Stability and Ion Pair Formation in Magnesium Electrolytes from First-Principles Quantum Mechanics and Classical Molecular Dynamics. Journal of the American Chemical Society, 2015, 137, 3411-3420.	13.7	259
4	The influence of FEC on the solvation structure and reduction reaction of LiPF6/EC electrolytes and its implication for solid electrolyte interphase formation. Nano Energy, 2019, 64, 103881.	16.0	239
5	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
6	Elucidating the structure of the magnesium aluminum chloride complex electrolyte for magnesium-ion batteries. Energy and Environmental Science, 2015, 8, 3718-3730.	30.8	131
7	Solvation structure and energetics of electrolytes for multivalent energy storage. Physical Chemistry Chemical Physics, 2014, 16, 21941-21945.	2.8	124
8	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. Nano Energy, 2015, 12, 750-759.	16.0	121
9	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. Chemistry of Materials, 2017, 29, 3375-3379.	6.7	117
10	Concentration dependent electrochemical properties and structural analysis of a simple magnesium electrolyte: magnesium bis(trifluoromethane sulfonyl)imide in diglyme. RSC Advances, 2016, 6, 113663-113670.	3.6	65
11	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€”A Review. Topics in Current Chemistry, 2018, 376, 19.	5.8	61
12	Structure and Dynamics of Polysulfide Clusters in a Nonaqueous Solvent Mixture of 1,3-Dioxolane and 1,2-Dimethoxyethane. Chemistry of Materials, 2019, 31, 2308-2319.	6.7	54
13	The Interplay between Salt Association and the Dielectric Properties of Low Permittivity Electrolytes: The Case of LiPF₆ and LiAsF₆ in Dimethyl Carbonate. Journal of Physical Chemistry C, 2018, 122, 1990-1994.	3.1	43
14	Rapid Upcycling of Waste Polyethylene Terephthalate to Energy Storing Disodium Terephthalate Flowers with DFT Calculations. ACS Sustainable Chemistry and Engineering, 2020, 8, 6252-6262.	6.7	43
15	25Mg NMR and computational modeling studies of the solvation structures and molecular dynamics in magnesium based liquid electrolytes. Nano Energy, 2018, 46, 436-446.	16.0	37
16	Effects of Anion Mobility on Electrochemical Behaviors of Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2017, 29, 9023-9029.	6.7	35
17	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	3.1	26
18	Diffusional motion of redox centers in carbonate electrolytes. Journal of Chemical Physics, 2014, 141, 104509.	3.0	24

#	Article	IF	Citations
19	Computational screening of electrolyte materials: status quo and open problems. Current Opinion in Chemical Engineering, 2019, 23, 58-69.	7.8	23
20	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€"A Review. Topics in Current Chemistry Collections, 2018, , 79-124.	0.5	14
21	Dipotassium terephthalate as promising potassium storing anode with DFT calculations. Materials Today Energy, 2020, 17, 100454.	4.7	12
22	Role of a Multivalent Ionâ€"Solvent Interaction on Restricted Mg²⁺ Diffusion in Dimethoxyethane Electrolytes. Journal of Physical Chemistry B, 2021, 125, 12574-12583.	2.6	7
23	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. Nature Computational Science, 2022, 2, 112-122.	8.0	4
24	Ab initio Study of Atomic Structure and Electronic Properties of Different Phases of Polymorphic Ag 2 S. Physica Status Solidi (B): Basic Research, 0, , 2100617.	1.5	0