

Nav Nidhi Rajput

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9450935/publications.pdf>

Version: 2024-02-01

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	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. <i>Nature Computational Science</i> , 2022, 2, 112-122.	8.0	4
2	Role of a Multivalent Ionâ€“Solvent Interaction on Restricted Mg ²⁺ Diffusion in Dimethoxyethane Electrolytes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12574-12583.	2.6	7
3	Rapid Upcycling of Waste Polyethylene Terephthalate to Energy Storing Disodium Terephthalate Flowers with DFT Calculations. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 6252-6262.	6.7	43
4	Dipotassium terephthalate as promising potassium storing anode with DFT calculations. <i>Materials Today Energy</i> , 2020, 17, 100454.	4.7	12
5	The influence of FEC on the solvation structure and reduction reaction of LiPF ₆ /EC electrolytes and its implication for solid electrolyte interphase formation. <i>Nano Energy</i> , 2019, 64, 103881.	16.0	239
6	Computational screening of electrolyte materials: status quo and open problems. <i>Current Opinion in Chemical Engineering</i> , 2019, 23, 58-69.	7.8	23
7	Structure and Dynamics of Polysulfide Clusters in a Nonaqueous Solvent Mixture of 1,3-Dioxolane and 1,2-Dimethoxyethane. <i>Chemistry of Materials</i> , 2019, 31, 2308-2319.	6.7	54
8	²⁵ Mg NMR and computational modeling studies of the solvation structures and molecular dynamics in magnesium based liquid electrolytes. <i>Nano Energy</i> , 2018, 46, 436-446.	16.0	37
9	The Interplay between Salt Association and the Dielectric Properties of Low Permittivity Electrolytes: The Case of LiPF ₆ and LiAsF ₆ in Dimethyl Carbonate. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1990-1994.	3.1	43
10	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€“A Review. <i>Topics in Current Chemistry</i> , 2018, 376, 19.	5.8	61
11	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€“A Review. <i>Topics in Current Chemistry Collections</i> , 2018, , 79-124.	0.5	14
12	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. <i>Chemistry of Materials</i> , 2017, 29, 3375-3379.	6.7	117
13	Non-encapsulation approach for high-performance Liâ€“S batteries through controlled nucleation and growth. <i>Nature Energy</i> , 2017, 2, 813-820.	39.5	326
14	Effects of Anion Mobility on Electrochemical Behaviors of Lithiumâ€“Sulfur Batteries. <i>Chemistry of Materials</i> , 2017, 29, 9023-9029.	6.7	35
15	Computational Design of New Magnesium Electrolytes with Improved Properties. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16126-16136.	3.1	26
16	Concentration dependent electrochemical properties and structural analysis of a simple magnesium electrolyte: magnesium bis(trifluoromethane sulfonyl)imide in diglyme. <i>RSC Advances</i> , 2016, 6, 113663-113670.	3.6	65
17	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 283-291.	4.6	276
18	The Coupling between Stability and Ion Pair Formation in Magnesium Electrolytes from First-Principles Quantum Mechanics and Classical Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2015, 137, 3411-3420.	13.7	259

#	ARTICLE	IF	CITATIONS
19	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. <i>Nano Energy</i> , 2015, 12, 750-759.	16.0	121
20	The Electrolyte Genome project: A big data approach in battery materials discovery. <i>Computational Materials Science</i> , 2015, 103, 56-67.	3.0	150
21	Elucidating the structure of the magnesium aluminum chloride complex electrolyte for magnesium-ion batteries. <i>Energy and Environmental Science</i> , 2015, 8, 3718-3730.	30.8	131
22	Diffusional motion of redox centers in carbonate electrolytes. <i>Journal of Chemical Physics</i> , 2014, 141, 104509.	3.0	24
23	Solvation structure and energetics of electrolytes for multivalent energy storage. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21941-21945.	2.8	124
24	Ab initio Study of Atomic Structure and Electronic Properties of Different Phases of Polymorphic Ag ₂ S. <i>Physica Status Solidi (B): Basic Research</i> , 0, , 2100617.	1.5	0