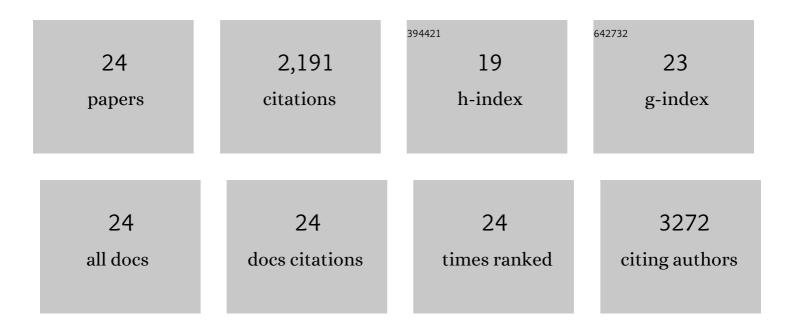
## Nav Nidhi Rajput

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. Nature Computational Science, 2022, 2, 112-122.	8.0	4
2	Role of a Multivalent Ion–Solvent Interaction on Restricted Mg <sup>2+</sup> Diffusion in Dimethoxyethane Electrolytes. Journal of Physical Chemistry B, 2021, 125, 12574-12583.	2.6	7
3	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
4	Dipotassium terephthalate as promising potassium storing anode with DFT calculations. Materials Today Energy, 2020, 17, 100454.	4.7	12
5	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
6	Computational screening of electrolyte materials: status quo and open problems. Current Opinion in Chemical Engineering, 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. Chemistry of Materials, 2019, 31, 2308-2319.	6.7	54
8	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
9	The Interplay between Salt Association and the Dielectric Properties of Low Permittivity Electrolytes: The Case of LiPF <sub>6</sub> and LiAsF <sub>6</sub> in Dimethyl Carbonate. Journal of Physical Chemistry C, 2018, 122, 1990-1994.	3.1	43
10	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytes—A Review. Topics in Current Chemistry, 2018, 376, 19.	5.8	61
11	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytes—A Review. Topics in Current Chemistry Collections, 2018, , 79-124.	O.5	14
12	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
13	Non-encapsulation approach for high-performance Li–S batteries through controlled nucleation and growth. Nature Energy, 2017, 2, 813-820.	39.5	326
14	Effects of Anion Mobility on Electrochemical Behaviors of Lithium–Sulfur Batteries. Chemistry of Materials, 2017, 29, 9023-9029.	6.7	35
15	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 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. RSC Advances, 2016, 6, 113663-113670.	3.6	65
17	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 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. Journal of the American Chemical Society, 2015, 137, 3411-3420.	13.7	259

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#	Article	IF	CITATIONS
19	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. Nano Energy, 2015, 12, 750-759.	16.0	121
20	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
21	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
22	Diffusional motion of redox centers in carbonate electrolytes. Journal of Chemical Physics, 2014, 141, 104509.	3.0	24
23	Solvation structure and energetics of electrolytes for multivalent energy storage. Physical Chemistry Chemical Physics, 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. Physica Status Solidi (B): Basic Research, 0, , 2100617.	1.5	0