Anirban Mondal

List of Publications by Year
in descending order

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26 papers	1,026 citations	516710 16 h-index	526287 27 g-index
27 all docs	27 docs citations	27 times ranked	1567 citing authors

#	Article	IF	Citations
1	Predicting chemical reaction equilibria in molten carbonate fuel cells via molecular simulations. AICHE Journal, 2021, 67, e16988.	3.6	8
2	First-Principles Modeling of Transport Mechanisms in Carbonateâ€“Hydroxide Electrolytes. Journal of Physical Chemistry C, 2021, 125, 4412-4422.	3.1	3
3	Molecular library of OLED host materialsâ€”Evaluating the multiscale simulation workflow. Chemical Physics Reviews, 2021, 2, .	5.7	24
4	Transport and Interfacial Properties of Mixed Molten Carbonate/Hydroxide Electrolytes by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 23532-23540.	3.1	7
5	Molecular simulation of liquidâ€“vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models. Journal of Chemical Physics, 2020, 153, 024501.	3.0	10
6	Genetic Algorithm Driven Force Field Parameterization for Molten Alkali-Metal Carbonate and Hydroxide Salts. Journal of Chemical Theory and Computation, 2020, 16, 5736-5746.	5.3	12
7	Electron Trapping in Conjugated Polymers. Chemistry of Materials, 2019, 31, 6380-6386.	6.7	70
8	Perspectives of Unicolored Phosphorâ€Sensitized Fluorescence. Advanced Electronic Materials, 2019, 5, 1900646.	5.1	21
9	A window to trap-free charge transport in organic semiconducting thin films. Nature Materials, 2019, 18, 1182-1186.	27.5	131
10	Selfâ€Organization and Charge Transport Properties of Selenium and Tellurium Analogues of Polythiophene. Macromolecular Rapid Communications, 2019, 40, e1800596.	3.9	18
11	Universal strategy for Ohmic hole injection into organic semiconductors with high ionization energies. Nature Materials, 2018, 17, 329-334.	27.5	168
12	Unicolored phosphor-sensitized fluorescence for efficient and stable blue OLEDs. Nature Communications, 2018, 9, 4990.	12.8	107
13	Rigorous Characterization and Predictive Modeling of Hole Transport in Amorphous Organic Semiconductors. Advanced Electronic Materials, 2018, 4, 1800366.	5.1	29
14	Molecular dynamics simulations of ammonium/phosphonium-based protic ionic liquids: influence of alkyl to aryl group. Physical Chemistry Chemical Physics, 2018, 20, 19268-19275.	2.8	9
15	Charge Environment and Hydrogen Bond Dynamics in Binary Ionic Liquid Mixtures: A Computational Study. Journal of Physical Chemistry Letters, 2018, 9, 3511-3516.	4.6	13
16	Recent advances in modeling green solvents. Current Opinion in Green and Sustainable Chemistry, 2017, 5, 37-43.	5.9	38
17	Molecular Dynamics Investigation of Efficient SO2 Absorption by Anion-Functionalized Ionic Liquids. Journal of Chemical Sciences, 2017, 129, 859-872.	1.5	7
18	Understanding SO₂ Capture by Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 4457-4466.	2.6	47

#	Article	IF	Citations
19	Proton Hopping Mechanisms in a Protic Organic Ionic Plastic Crystal. Journal of Physical Chemistry C, 2016, 120, 22903-22909.	3.1	11
20	Thermal phase behavior and ion hopping in a 1,2,4-triazolium perfluorobutanesulfonate protic organic ionic plastic crystal. Physical Chemistry Chemical Physics, 2016, 18, 2047-2053.	2.8	11
21	Atomistic simulations of ammonium-based protic ionic liquids: steric effects on structure, low frequency vibrational modes and electrical conductivity. Physical Chemistry Chemical Physics, 2015, 17, 4625-4633.	2.8	36
22	Vibrational Signatures of Cationâ€“Anion Hydrogen Bonding in Ionic Liquids: A Periodic Density Functional Theory and Molecular Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 1994-2002.	2.6	20
23	Dissolution of Cellulose in Room Temperature Ionic Liquids: Anion Dependence. Journal of Physical Chemistry B, 2015, 119, 1654-1659.	2.6	44
24	A Refined All-Atom Potential for Imidazolium-Based Room Temperature Ionic Liquids: Acetate, Dicyanamide, and Thiocyanate Anions. Journal of Physical Chemistry B, 2015, 119, 11041-11051.	2.6	39
25	A Molecular Dynamics Study of Collective Transport Properties of Imidazolium-Based Room-Temperature Ionic Liquids. Journal of Chemical & Engineering Data, 2014, 59, 3061-3068.	1.9	34
26	Quantitative Prediction of Physical Properties of Imidazolium Based Room Temperature Ionic Liquids through Determination of Condensed Phase Site Charges: A Refined Force Field. Journal of Physical Chemistry B, 2014, 118, 3409-3422.	2.6	106