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List of Publications by Year
in descending order

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34 papers	1,409 citations	394421 19 h-index	377865 34 g-index
36 all docs	36 docs citations	36 times ranked	1589 citing authors

#	Article	IF	Citations
1	Prediction and Interpretation of Polymer Properties Using the Graph Convolutional Network. ACS Polymers Au, 2022, 2, 213-222.	4.1	24
2	A Computer Simulation Study of Thermal and Mechanical Properties of Poly(Ionic Liquid)s. Membranes, 2022, 12, 450.	3.0	0
3	Controlling Gas Generation of Li-Ion Battery through Divinyl Sulfone Electrolyte Additive. International Journal of Molecular Sciences, 2022, 23, 7328.	4.1	1
4	Comparison of Machine Learning Methods towards Developing Interpretable Polyamide Property Prediction. Polymers, 2021, 13, 3653.	4.5	8
5	First-principles study of the surface reactions of aminosilane precursors over WO₃(001) during atomic layer deposition of SiO₂. RSC Advances, 2020, 10, 16584-16592.	3.6	3
6	Computer simulation study of fluorocarbon phosphate surfactant based aqueous reverse micelle in supercritical CO₂: roles of surfactant functional groups, ionic strength, and phase changes in CO₂. Physical Chemistry Chemical Physics, 2020, 22, 3434-3445.	2.8	3
7	Reductive reactions via excess Li in mixture electrolytes of Li ion batteries: an ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2019, 21, 5489-5498.	2.8	9
8	Computer simulation study of the solvation of lithium ions in ternary mixed carbonate electrolytes: free energetics, dynamics, and ion transport. Physical Chemistry Chemical Physics, 2018, 20, 28649-28657.	2.8	18
9	Effects of Alkyl Chain Length on Interfacial Structure and Differential Capacitance in Graphene Supercapacitors: A Molecular Dynamics Simulation Study. Electrochimica Acta, 2017, 247, 634-645.	5.2	47
10	Excitation-energy dependence of solvation dynamics in room-temperature ionic liquids. Journal of Chemical Physics, 2016, 145, 044502.	3.0	6
11	Atomic layer deposition of diisopropylaminosilane on WO3(001) and W(110): a density functional theory study. Physical Chemistry Chemical Physics, 2016, 18, 29139-29146.	2.8	3
12	Theoretical study of interactions of a Li⁺(CF₃SO₂)₂N^{â^'} ion pair with CR₃(OCR₂CR₂)_nOCR₃ (R = H or F). Physical Chemistry Chemical Physics, 2016, 18, 6754-6762.	2.8	14
13	Computer Simulation Study of Graphene Oxide Supercapacitors: Charge Screening Mechanism. Journal of Physical Chemistry Letters, 2016, 7, 1180-1186.	4.6	38
14	Influence of polyvinylpyrrolidone (PVP) capping layer on silver nanowire networks: theoretical and experimental studies. RSC Advances, 2016, 6, 30972-30977.	3.6	63
15	Modulation of the Dirac Point Voltage of Graphene by Ion-Gel Dielectrics and Its Application to Soft Electronic Devices. ACS Nano, 2015, 9, 602-611.	14.6	28
16	Graphene Oxide Supercapacitors: A Computer Simulation Study. Journal of Physical Chemistry C, 2014, 118, 18472-18480.	3.1	60
17	Dielectric Relaxation and Solvation Dynamics in a Room-Temperature Ionic Liquid: Temperature Dependence. Journal of Physical Chemistry B, 2013, 117, 11743-11752.	2.6	29
18	Graphene-based supercapacitors in the parallel-plate electrode configuration: Ionic liquidsversus organic electrolytes. Faraday Discussions, 2012, 154, 249-263.	3.2	79

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19	Solvation of a Small Metal-Binding Peptide in Room-Temperature Ionic Liquids. Bulletin of the Korean Chemical Society, 2012, 33, 3601-3606.	1.9	6
20	Graphene-Based Supercapacitors: A Computer Simulation Study. Journal of Physical Chemistry C, 2011, 115, 23574-23583.	3.1	104
21	Carbon nanotubes in benzene: internal and external solvation. Physical Chemistry Chemical Physics, 2011, 13, 3969.	2.8	22
22	MD Study of Solvation in the Mixture of a Room-Temperature Ionic Liquid and CO₂. Journal of Physical Chemistry B, 2010, 114, 10160-10170.	2.6	28
23	Nanoporous Carbon Supercapacitors in an Ionic Liquid: A Computer Simulation Study. ACS Nano, 2010, 4, 2345-2355.	14.6	267
24	Adiabatic Electron Transfer in a Room-Temperature Ionic Liquid: Reaction Dynamics and Kinetics. Journal of Physical Chemistry B, 2009, 113, 12964-12972.	2.6	32
25	Solvation of Carbon Nanotubes in a Room-Temperature Ionic Liquid. ACS Nano, 2009, 3, 1693-1702.	14.6	140
26	Electron-Transfer Reactions in Supercritical Water. Journal of Physical Chemistry B, 2008, 112, 585-594.	2.6	4
27	MD Study of S_N1 Reactivity of 2-Chloro-2-methylpropane in the Room-Temperature Ionic Liquid 1-Ethyl-3-methylimidazolium Hexafluorophosphate. Journal of Physical Chemistry B, 2008, 112, 2637-2643.	2.6	11
28	Dielectric Relaxation, Ion Conductivity, Solvent Rotation, and Solvation Dynamics in a Room-Temperature Ionic Liquid. Journal of Physical Chemistry B, 2008, 112, 11028-11038.	2.6	91
29	Effects of Solute Electronic Polarizability on Solvation in a Room-Temperature Ionic Liquidâ€. Journal of Physical Chemistry B, 2007, 111, 4920-4925.	2.6	53
30	Solvation, Solute Rotation and Vibration Relaxation, and Electron-Transfer Reactions in Room-Temperature Ionic Liquids. Accounts of Chemical Research, 2007, 40, 1130-1137.	15.6	78
31	Free Energy and Dynamics of Electron-Transfer Reactions in a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2007, 111, 4510-4519.	2.6	64
32	Vibrational energy relaxation of a diatomic molecule in a room-temperature ionic liquid. Journal of Chemical Physics, 2006, 125, 024507.	3.0	15
33	Rotational dynamics of a diatomic solute in the room-temperature ionic liquid 1-ethyl-3-methylimidazolium hexafluorophosphate. Journal of Chemical Physics, 2006, 125, 061102.	3.0	36
34	Solvation in supercritical water. Journal of Chemical Physics, 2006, 124, 204504.	3.0	20