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List of Publications by Year
in descending order

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42	1,417	304368	329751
papers	citations	22 h-index	37 g-index

45	45	45	1576
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Capacitance of Carbon Nanotube/Graphene Composite Electrodes with [BMIM⁺][BF₄^{â€“}]/Acetonitrile: Fixed Voltage Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2022, 126, 5822-5837.	1.5	10
2	DFT-based QM/MM with particle-mesh Ewald for direct, long-range electrostatic embedding. Journal of Chemical Physics, 2022, 156, 174105.	1.2	6
3	Quantized Electrodes: Atomic Palladium and Gold in Polyaniline. ChemElectroChem, 2021, 8, 1766-1774.	1.7	4
4	Deep Eutectic Solvents: Molecular Simulations with a First-Principles Polarizable Force Field. Journal of Physical Chemistry B, 2021, 125, 7177-7186.	1.2	13
5	Physics-based, neural network force fields for reactive molecular dynamics: Investigation of carbene formation from [EMIM+][OAcâ^]. Journal of Chemical Physics, 2021, 155, 104112.	1.2	6
6	Structureâ€“Capacitance Relationships of Graphene/Ionic Liquid Electrolyte Double Layers. Journal of Physical Chemistry C, 2021, 125, 20204-20218.	1.5	16
7	A Transferable Polarizable Force Field for Urea Crystals and Aqueous Solutions. Journal of Physical Chemistry B, 2020, 124, 7475-7483.	1.2	12
8	Proton Transport in [BMIM⁺][BF₄^{â€“}]/Water Mixtures Near the Percolation Threshold. Journal of Physical Chemistry B, 2020, 124, 5957-5970.	1.2	6
9	Interference of electrical double layers: Confinement effects on structure, dynamics, and screening of ionic liquids. Journal of Chemical Physics, 2020, 152, 074709.	1.2	29
10	Tuning Water Networks via Ionic Liquid/Water Mixtures. International Journal of Molecular Sciences, 2020, 21, 403.	1.8	23
11	Inner Layer Capacitance of Organic Electrolytes from Constant Voltage Molecular Dynamics. Journal of Physical Chemistry C, 2020, 124, 2907-2922.	1.5	25
12	A nanoconfined iron(<scp>iii</scp>) fluoride cathode in a NaDFOB electrolyte: towards high-performance sodium-ion batteries. Journal of Materials Chemistry A, 2020, 8, 4091-4098.	5.2	28
13	Free energy barriers for TMEA+, TMA+, and BF4- ion diffusion through nanoporous carbon electrodes. Carbon, 2020, 161, 550-561.	5.4	11
14	On the Miscibility and Immiscibility of Ionic Liquids and Water. Journal of Physical Chemistry B, 2019, 123, 5343-5356.	1.2	29
15	Understanding the Properties of Ionic Liquids: Electrostatics, Structure Factors, and Their Sum Rules. Journal of Physical Chemistry B, 2019, 123, 3499-3512.	1.2	48
16	Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-NosÃ©â€“Hoover Thermostat. Journal of Physical Chemistry Letters, 2019, 10, 7523-7530.	2.1	29
17	Polarization Effects in Binary [BMIM⁺][BF₄^{â€“}]/1,2-Dichloroethane, Acetone, Acetonitrile, and Water Electrolytes. Journal of Physical Chemistry B, 2018, 122, 4345-4355.	1.2	33
18	Ab Initio Force Fields for Organic Anions: Properties of [BMIM][TFSI], [BMIM][FSI], and [BMIM][OTf] Ionic Liquids. Journal of Physical Chemistry B, 2018, 122, 4101-4114.	1.2	45

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19	Grotthuss Transport of Iodide in EMIM/I₃ Ionic Crystal. Journal of Physical Chemistry B, 2018, 122, 250-257.	1.2	17
20	Ion Correlation and Collective Dynamics in BMIM/BF₄-Based Organic Electrolytes: From Dilute Solutions to the Ionic Liquid Limit. Journal of Physical Chemistry B, 2018, 122, 7154-7169.	1.2	60
21	Influence of Electronic Polarization on the Structure of Ionic Liquids. Journal of Physical Chemistry Letters, 2018, 9, 4765-4770.	2.1	54
22	Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM⁺BF₄^{â€“}: A Microsecond Computer Simulation Study Using ab Initio Force Fields. Macromolecules, 2018, 51, 5336-5345.	2.2	16
23	Coupling between the Dynamics of Water and Surfactants in Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2017, 121, 5048-5057.	1.2	3
24	Electrostatic Interactions Govern â€œOdd/Evenâ€•Effects in Water-Induced Gemini Surfactant Self-Assembly. Journal of Physical Chemistry B, 2017, 121, 565-576.	1.2	16
25	Proton Diffusion through Bilayer Pores. Journal of Physical Chemistry B, 2017, 121, 9247-9259.	1.2	2
26	Importance of hydrophobic traps for proton diffusion in lyotropic liquid crystals. Journal of Chemical Physics, 2016, 144, 094705.	1.2	6
27	Comment on â€œIsolating the non-polar contributions to the intermolecular potential for water-alkane interactionsâ€•[J. Chem. Phys. 141, 064905 (2014)]. Journal of Chemical Physics, 2016, 144, 137101.	1.2	14
28	Ab Initio Force Fields for Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 7024-7036.	1.2	76
29	Next-Generation Force Fields from Symmetry-Adapted Perturbation Theory. Annual Review of Physical Chemistry, 2016, 67, 467-488.	4.8	66
30	Dynamics of Water in Gemini Surfactant-Based Lyotropic Liquid Crystals. Journal of Physical Chemistry B, 2016, 120, 10860-10868.	1.2	12
31	Conformational and Dynamic Properties of Poly(ethylene oxide) in an Ionic Liquid: Development and Implementation of a First-Principles Force Field. Journal of Physical Chemistry B, 2016, 120, 231-243.	1.2	21
32	First-Principles United Atom Force Field for the Ionic Liquid BMIM⁺BF₄^{â€“}: An Alternative to Charge Scaling. Journal of Physical Chemistry B, 2016, 120, 3560-3568.	1.2	68
33	Transferable Next-Generation Force Fields from Simple Liquids to Complex Materials. Accounts of Chemical Research, 2015, 48, 548-556.	7.6	71
34	Evaluation of Force Field Performance for High-Throughput Screening of Gas Uptake in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 3143-3152.	1.5	85
35	First-Principles Many-Body Force Fields from the Gas Phase to Liquid: A â€œUniversalâ€•Approach. Journal of Physical Chemistry B, 2014, 118, 8042-8053.	1.2	52
36	First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF₄]. Journal of Physical Chemistry Letters, 2014, 5, 2670-2674.	2.1	57

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37	Microscopic Origins of Enhanced Gas Adsorption and Selectivity in Mixed-Linker Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 17131-17142.	1.5	20
38	Physically-Motivated Force Fields from Symmetry-Adapted Perturbation Theory. Journal of Physical Chemistry A, 2013, 117, 2053-2066.	1.1	120
39	An efficient multi-scale lattice model approach to screening nano-porous adsorbents. Journal of Chemical Physics, 2012, 137, 244102.	1.2	11
40	Ab Initio, Physically Motivated Force Fields for CO₂ Adsorption in Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2012, 116, 1892-1903.	1.5	87
41	Robust, Transferable, and Physically Motivated Force Fields for Gas Adsorption in Functionalized Zeolitic Imidazolate Frameworks. Journal of Physical Chemistry C, 2012, 116, 14031-14039.	1.5	53
42	Physically Motivated, Robust, ab Initio Force Fields for CO₂and N₂. Journal of Physical Chemistry B, 2011, 115, 10054-10063.	1.2	51