Baofu Qiao

List of Publications by Year
in descending order

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52 papers	1,795 citations	218677 26 h-index	276875 41 g-index
55 all docs	55 docs citations	55 times ranked	2355 citing authors

#	Article	IF	Citations
1	Specific Ion Effects in Lanthanideâ€“Amphiphile Structures at the Airâ€“Water Interface and Their Implications for Selective Separation. ACS Applied Materials & Interfaces, 2022, 14, 7504-7512.	8.0	14
2	Acid-Base Equilibrium and Dielectric Environment Regulate Charge in Supramolecular Nanofibers. Frontiers in Chemistry, 2022, 10, 852164.	3.6	6
3	Functional enzymeâ€“polymer complexes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2119509119.	7.1	13
4	Origins of Clustering of Metalateâ€“Extractant Complexes in Liquidâ€“Liquid Extraction. ACS Applied Materials & Interfaces, 2021, 13, 24194-24206.	8.0	27
5	Origin of Proteolytic Stability of Peptide-Brush Polymers as Globular Proteomimetics. ACS Central Science, 2021, 7, 2063-2072.	11.3	10
6	Single-chain heteropolymers transport protons selectively and rapidly. Nature, 2020, 577, 216-220.	27.8	64
7	Homopolymer self-assembly of poly(propylene sulfone) hydrogels via dynamic noncovalent sulfoneâ€“sulfone bonding. Nature Communications, 2020, 11, 4896.	12.8	21
8	Insights into the Enhanced Catalytic Activity of Cytochrome c When Encapsulated in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2020, 142, 18576-18582.	13.7	73
9	Enhanced Binding of SARS-CoV-2 Spike Protein to Receptor by Distal Polybasic Cleavage Sites. ACS Nano, 2020, 14, 10616-10623.	14.6	89
10	Protein Surface Printer for Exploring Protein Domains. Journal of Chemical Information and Modeling, 2020, 60, 5255-5264.	5.4	2
11	PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. Molecules, 2020, 25, 1848.	3.8	5
12	Water follows polar and nonpolar protein surface domains. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19274-19281.	7.1	66
13	â€œMirrorâ€•like Protein Dimers Stabilized by Local Heterogeneity at Protein Surfaces. Journal of Physical Chemistry B, 2019, 123, 3907-3915.	2.6	13
14	Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. Soft Matter, 2019, 15, 9437-9451.	2.7	5
15	Ion association with tetra-n-alkylammonium cations stabilizes higher-oxidation-state neptunium dioxocations. Nature Communications, 2019, 10, 59.	12.8	20
16	Liquid worm-like and proto-micelles: water solubilization in amphiphileâ€“oil solutions. Physical Chemistry Chemical Physics, 2018, 20, 12908-12915.	2.8	17
17	Comparative CHARMM and AMOEBA Simulations of Lanthanide Hydration Energetics and Experimental Aqueous-Solution Structures. Journal of Chemical Theory and Computation, 2018, 14, 1781-1790.	5.3	28
18	All-Atom Molecular Dynamics Study of Waterâ€“Dodecane Interface in the Presence of Octanol. Journal of Physical Chemistry C, 2018, 122, 687-693.	3.1	12

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19	Random heteropolymers preserve protein function in foreign environments. Science, 2018, 359, 1239-1243.	12.6	196
20	Heavy Anionic Complex Creates a Unique Water Structure at a Soft Charged Interface. Journal of Physical Chemistry C, 2018, 122, 29228-29236.	3.1	29
21	Efficient encapsulation of proteins with random copolymers. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6578-6583.	7.1	34
22	Ion condensation onto selfâ€assembled nanofibers. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 901-906.	2.1	6
23	Water Dynamics from the Surface to the Interior of a Supramolecular Nanostructure. Journal of the American Chemical Society, 2017, 139, 8915-8921.	13.7	53
24	Ion Transport Mechanisms in Liquidâ€“Liquid Interface. Langmuir, 2017, 33, 6135-6142.	3.5	44
25	Subtle Effects of Aliphatic Alcohol Structure on Water Extraction and Solute Aggregation in Biphasic Water/n-Dodecane. Langmuir, 2017, 33, 3776-3786.	3.5	15
26	Two-Step Adsorption of PtCl62â€“ Complexes at a Charged Langmuir Monolayer: Role of Hydration and Ion Correlations. Journal of Physical Chemistry C, 2017, 121, 25377-25383.	3.1	28
27	Complexation Enhancement Drives Waterâ€toâ€Oil Ion Transport: A Simulation Study. Chemistry - A European Journal, 2017, 23, 427-436.	3.3	11
28	The Lanthanide Contraction beyond Coordination Chemistry. Chemistry - A European Journal, 2016, 22, 6899-6904.	3.3	37
29	Aggregation of Heteropolyanions in Aqueous Solutions Exhibiting Short-Range Attractions and Long-Range Repulsions. Journal of Physical Chemistry C, 2016, 120, 1317-1327.	3.1	37
30	Atomistic Simulation of Oligoelectrolyte Multilayers Growth. , 2016, , 215-228.		1
31	Molecular Origins of Mesoscale Ordering in a Metalloamphiphile Phase. ACS Central Science, 2015, 1, 493-503.	11.3	44
32	Generic force fields for ionic liquids. Journal of Molecular Liquids, 2014, 192, 32-37.	4.9	32
33	Liquidâ€“liquid phase separation of ionic liquids in solutions: Ionic liquids with the triflat anion solved in aryl halides. Journal of Molecular Liquids, 2014, 192, 127-136.	4.9	20
34	Structures, Dynamics, and Water Permeation Free Energy across Bilayers of Lipid A and Its Analog Studied with Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2014, 118, 13202-13209.	2.6	20
35	Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. Soft Materials, 2014, 12, S14-S21.	1.7	13
36	How Hydrogen Bonds Affect the Growth of Reverse Micelles around Coordinating Metal Ions. Journal of Physical Chemistry Letters, 2014, 5, 1440-1444.	4.6	63

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37	Driving Force for Water Permeation Across Lipid Membranes. Journal of Physical Chemistry Letters, 2013, 4, 3233-3237.	4.6	32
38	Driving Force for Crystallization of Anionic Lipid Membranes Revealed by Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 5073-5080.	2.6	16
39	Potassium ions in the cavity of a KcsA channel model. Physical Review E, 2013, 88, 062712.	2.1	6
40	Crystalline polymorphism induced by charge regulation in ionic membranes. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 16309-16314.	7.1	40
41	Properties of water in the interfacial region of a polyelectrolyte bilayer adsorbed onto a substrate studied by computer simulations. Physical Chemistry Chemical Physics, 2012, 14, 11425.	2.8	13
42	Molecular Crystallization Controlled by pH Regulates Mesoscopic Membrane Morphology. ACS Nano, 2012, 6, 10901-10909.	14.6	56
43	An atomistic study of a poly(styrene sulfonate)/poly(diallyldimethylammonium) bilayer: the role of surface properties and charge reversal. Physical Chemistry Chemical Physics, 2011, 13, 16336.	2.8	21
44	Atomistic Study of Surface Effects on Polyelectrolyte Adsorption: Case Study of a Poly(styrenesulfonate) Monolayer. Macromolecules, 2011, 44, 1707-1718.	4.8	33
45	Structure of 1-Butylpyridinium Tetrafluoroborate Ionic Liquid: Quantum Chemistry and Molecular Dynamic Simulation Studies. Journal of Physical Chemistry A, 2010, 114, 3990-3996.	2.5	43
46	Poly(styrenesulfonate)â^'Poly(diallyldimethylammonium) Mixtures: Toward the Understanding of Polyelectrolyte Complexes and Multilayers via Atomistic Simulations. Macromolecules, 2010, 43, 7828-7838.	4.8	45
47	Description of Ionic Surfactant/Water System by Adjusting Mesoscopic Parameters. Journal of Physical Chemistry B, 2009, 113, 8854-8859.	2.6	17
48	Understanding polyelectrolyte multilayers: an open challenge for simulations. Soft Matter, 2009, 5, 4412.	2.7	54
49	A comparative study of two classical force fields on statics and dynamics of [EMIM][BF4] investigated via molecular dynamics simulations. Journal of Chemical Physics, 2008, 129, 224501.	3.0	89
50	Effect of Anions on Static Orientational Correlations, Hydrogen Bonds, and Dynamics in Ionic Liquids:â€‰ A Simulational Study. Journal of Physical Chemistry B, 2008, 112, 1743-1751.	2.6	111
51	Study of 1,3-dimethylimidazolium chloride with electronic structure methods and force field approaches. Journal of Chemical Physics, 2008, 129, 174503.	3.0	33
52	A theory of polymer solutions without the mean-field approximation in Flory-Huggins theory. Journal of Chemical Physics, 2004, 121, 4968-4973.	3.0	12