# Baofu Qiao

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1854576/publications.pdf

Version: 2024-02-01

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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 | Random heteropolymers preserve protein function in foreign environments. Science, 2018, 359, 1239-1243. | 12.6 | 196 |
| 2 | 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 |
| 3 | 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 |
| 4 | Enhanced Binding of SARS-CoV-2 Spike Protein to Receptor by Distal Polybasic Cleavage Sites. ACS Nano, 2020, 14, 10616-10623. | 14.6 | 89 |
| 5 | 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 |
| 6 | 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 |
| 7 | Single-chain heteropolymers transport protons selectively and rapidly. Nature, 2020, 577, 216-220. | 27.8 | 64 |
| 8 | 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 |
| 9 | Molecular Crystallization Controlled by pH Regulates Mesoscopic Membrane Morphology. ACS Nano, 2012, 6, 10901-10909. | 14.6 | 56 |
| 10 | Understanding polyelectrolyte multilayers: an open challenge for simulations. Soft Matter, 2009, 5, 4412. | 2.7 | 54 |
| 11 | 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 |
| 12 | 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 |
| 13 | Molecular Origins of Mesoscale Ordering in a Metalloamphiphile Phase. ACS Central Science, 2015, 1, 493-503. | 11.3 | 44 |
| 14 | Ion Transport Mechanisms in Liquidâ€“Liquid Interface. Langmuir, 2017, 33, 6135-6142. | 3.5 | 44 |
| 15 | 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 |
| 16 | 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 |
| 17 | The Lanthanide Contraction beyond Coordination Chemistry. Chemistry - A European Journal, 2016, 22, 6899-6904. | 3.3 | 37 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Study of 1,3-dimethylimidazolium chloride with electronic structure methods and force field approaches. Journal of Chemical Physics, 2008, 129, 174503. | 3.0 | 33 |
| 21 | Atomistic Study of Surface Effects on Polyelectrolyte Adsorption: Case Study of a Poly(styrenesulfonate) Monolayer. Macromolecules, 2011, 44, 1707-1718. | 4.8 | 33 |
| 22 | Driving Force for Water Permeation Across Lipid Membranes. Journal of Physical Chemistry Letters, 2013, 4, 3233-3237. | 4.6 | 32 |
| 23 | Generic force fields for ionic liquids. Journal of Molecular Liquids, 2014, 192, 32-37. | 4.9 | 32 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | Origins of Clustering of Metalateâ€“Extractant Complexes in Liquidâ€“Liquid Extraction. ACS Applied Materials & Interfaces, 2021, 13, 24194-24206. | 8.0 | 27 |
| 28 | 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 |
| 29 | Homopolymer self-assembly of poly(propylene sulfone) hydrogels via dynamic noncovalent sulfoneâ€“sulfone bonding. Nature Communications, 2020, 11, 4896. | 12.8 | 21 |
| 30 | 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 |
| 31 | 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 |
| 32 | Ion association with tetra-n-alkylammonium cations stabilizes higher-oxidation-state neptunium dioxocations. Nature Communications, 2019, 10, 59. | 12.8 | 20 |
| 33 | Description of Ionic Surfactant/Water System by Adjusting Mesoscopic Parameters. Journal of Physical Chemistry B, 2009, 113, 8854-8859. | 2.6 | 17 |
| 34 | Liquid worm-like and proto-micelles: water solubilization in amphiphileâ€“oil solutions. Physical Chemistry Chemical Physics, 2018, 20, 12908-12915. | 2.8 | 17 |
| 35 | Driving Force for Crystallization of Anionic Lipid Membranes Revealed by Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 5073-5080. | 2.6 | 16 |
| 36 | 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 |

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|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. Soft Materials, 2014, 12, S14-S21. | 1.7 | 13 |
| 40 | â€œMirrorâ€•like Protein Dimers Stabilized by Local Heterogeneity at Protein Surfaces. Journal of Physical Chemistry B, 2019, 123, 3907-3915. | 2.6 | 13 |
| 41 | Functional enzymeâ€“polymer complexes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2119509119. | 7.1 | 13 |
| 42 | 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 |
| 43 | 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 |
| 44 | Complexation Enhancement Drives Waterâ€toâ€Oil Ion Transport: A Simulation Study. Chemistry - A European Journal, 2017, 23, 427-436. | 3.3 | 11 |
| 45 | Origin of Proteolytic Stability of Peptide-Brush Polymers as Globular Proteomimetics. ACS Central Science, 2021, 7, 2063-2072. | 11.3 | 10 |
| 46 | Potassium ions in the cavity of a KcsA channel model. Physical Review E, 2013, 88, 062712. | 2.1 | 6 |
| 47 | Ion condensation onto selfâ€assembled nanofibers. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 901-906. | 2.1 | 6 |
| 48 | Acid-Base Equilibrium and Dielectric Environment Regulate Charge in Supramolecular Nanofibers. Frontiers in Chemistry, 2022, 10, 852164. | 3.6 | 6 |
| 49 | Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. Soft Matter, 2019, 15, 9437-9451. | 2.7 | 5 |
| 50 | PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. Molecules, 2020, 25, 1848. | 3.8 | 5 |
| 51 | Protein Surface Printer for Exploring Protein Domains. Journal of Chemical Information and Modeling, 2020, 60, 5255-5264. | 5.4 | 2 |
| 52 | Atomistic Simulation of Oligoelectrolyte Multilayers Growth. , 2016, , 215-228. | | 1 |