J Alfredo Freites

List of Publications by Year
in descending order

70 papers	5,530 citations	304368 22 h-index	155451 55 g-index
70 all docs	70 docs citations	70 times ranked	7265 citing authors

#	Article	IF	Citations
1	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	1.2	3,676
2	Interface connections of a transmembrane voltage sensor. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 15059-15064.	3.3	208
3	Structure and hydration of membranes embedded with voltage-sensing domains. Nature, 2009, 462, 473-479.	13.7	175
4	Arginine in Membranes: The Connection Between Molecular Dynamics Simulations and Translocon-Mediated Insertion Experiments. Journal of Membrane Biology, 2011, 239, 35-48.	1.0	104
5	Allosteric mechanism of water-channel gating by Ca2+â€“calmodulin. Nature Structural and Molecular Biology, 2013, 20, 1085-1092.	3.6	102
6	A Voltage-Sensor Water Pore. Biophysical Journal, 2006, 91, L90-L92.	0.2	89
7	Opening and closing of the periplasmic gate in lactose permease. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 3774-3778.	3.3	84
8	Acyl-Chain Methyl Distributions of Liquid-Ordered and -Disordered Membranes. Biophysical Journal, 2011, 100, 1455-1462.	0.2	70
9	Water wires in atomistic models of the Hv1 proton channel. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 286-293.	1.4	67
10	Separating Instability from Aggregation Propensity in Î³S-Crystallin Variants. Biophysical Journal, 2011, 100, 498-506.	0.2	64
11	Molecular Biophysics of Orai Store-Operated Ca2+ Channels. Biophysical Journal, 2015, 108, 237-246.	0.2	64
12	Proton-Coupled Dynamics in Lactose Permease. Structure, 2012, 20, 1893-1904.	1.6	53
13	YidC Insertase of Escherichia coli: Water Accessibility and Membrane Shaping. Structure, 2017, 25, 1403-1414.e3.	1.6	50
14	Dynamics of SecY Translocons with Translocation-Defective Mutations. Structure, 2010, 18, 847-857.	1.6	47
15	Outer membrane phospholipase A in phospholipid bilayers: A model system for concerted computational and experimental investigations of amino acid side chain partitioning into lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 126-134.	1.4	39
16	Molecular Dynamics Simulations of a Pulmonary Surfactant Protein B Peptide in a Lipid Monolayer. Biophysical Journal, 2003, 84, 2169-2180.	0.2	36
17	Specific cation effects at aqueous solutionâ^'vapor interfaces: Surfactant-like behavior of Li ⁺ revealed by experiments and simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13363-13368.	3.3	34
18	Down-State Model of the Voltage-Sensing Domain of a Potassium Channel. Biophysical Journal, 2010, 98, 2857-2866.	0.2	33

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19	Interleaflet mixing and coupling in liquid-disordered phospholipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 354-362.	1.4	29
20	Voltage-dependent structural models of the human Hv1 proton channel from long-timescale molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 13490-13498.	3.3	29
21	Assembly and stability of Î±-helical membrane proteins. Soft Matter, 2012, 8, 7742.	1.2	28
22	Microscopic Origin of Gating Current Fluctuations in a Potassium Channel Voltage Sensor. Biophysical Journal, 2012, 102, L44-L46.	0.2	28
23	Calmodulin Gates Aquaporin 0 Permeability through a Positively Charged Cytoplasmic Loop. Journal of Biological Chemistry, 2017, 292, 185-195.	1.6	26
24	Two transmembrane dimers of the bovine papillomavirus E5 oncoprotein clamp the PDGF Î² receptor in an active dimeric conformation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E7262-E7271.	3.3	26
25	Experimental and Simulation Studies of Aquaporin 0 Water Permeability and Regulation. Chemical Reviews, 2019, 119, 6015-6039.	23.0	25
26	Annexin A1 Interaction with a Zwitterionic Phospholipid Monolayer:Â A Fluorescence Microscopy Study. Langmuir, 2004, 20, 11674-11683.	1.6	22
27	Structural Plasticity in the Topology of the Membrane-Interacting Domain of HIV-1 gp41. Biophysical Journal, 2014, 106, 610-620.	0.2	22
28	Transmembrane helices containing a charged arginine are thermodynamically stable. European Biophysics Journal, 2017, 46, 627-637.	1.2	21
29	Increased hydrophobic surface exposure in the cataract-related G18V variant of human Î³S-crystallin. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 325-332.	1.1	20
30	Sequence comparison, molecular modeling, and network analysis predict structural diversity in cysteine proteases from the Cape sundew, Drosera capensis. Computational and Structural Biotechnology Journal, 2016, 14, 271-282.	1.9	19
31	Structural Dynamics of the S4 Voltage-Sensor Helix in Lipid Bilayers Lacking Phosphate Groups. Journal of Physical Chemistry B, 2011, 115, 8732-8738.	1.2	18
32	Interaction of Water Vapor with the Surfaces of Imidazolium-Based Ionic Liquid Nanoparticles and Thin Films. Journal of Physical Chemistry B, 2012, 116, 11255-11265.	1.2	18
33	Coupling between the voltage-sensing and pore domains in a voltage-gated potassium channel. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 1726-1736.	1.4	18
34	Voltage Sensing in Membranes: From Macroscopic Currents to Molecular Motions. Journal of Membrane Biology, 2015, 248, 419-430.	1.0	18
35	Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain. Journal of Membrane Biology, 2018, 251, 379-391.	1.0	18
36	Direct Evidence of Conformational Changes Associated with Voltage Gating in a Voltage Sensor Protein by Time-Resolved X-ray/Neutron Interferometry. Langmuir, 2014, 30, 4784-4796.	1.6	16

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37	Molecular Mechanism of Aggregation of the Cataract-Related Î³D-Crystallin W42R Variant from Multiscale Atomistic Simulations. Biochemistry, 2019, 58, 3691-3699.	1.2	16
38	Cooperativity and allostery in aquaporin 0 regulation by Ca2+. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 988-996.	1.4	16
39	Structural Characterization of the Voltage-Sensor Domain and Voltage-Gated K⁺-Channel Proteins Vectorially Oriented within a Single Bilayer Membrane at the Solid/Vapor and Solid/Liquid Interfaces via Neutron Interferometry. Langmuir, 2012, 28, 10504-10520.	1.6	14
40	Multi-Conformation Monte Carlo: A Method for Introducing Flexibility in Efficient Simulations of Many-Protein Systems. Journal of Physical Chemistry B, 2016, 120, 8115-8126.	1.2	12
41	Molecular Arrangement of a Mixture of Organosulfur Surfactants at the Aqueous Solutionâ€“Vapor Interface Studied by Photoelectron Intensity and Angular Distribution Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 8160-8170.	1.5	11
42	Atomistic Modeling of Ion Conduction through the Voltage-Sensing Domain of the Shaker K⁺ Ion Channel. Journal of Physical Chemistry B, 2017, 121, 3804-3812.	1.2	9
43	Synthesis and characterization of nanophase particles obtained by D.C. sputtering. Scripta Materialia, 2001, 44, 1883-1887.	2.6	8
44	Insights on small molecule binding to the Hv1 proton channel from free energy calculations with molecular dynamics simulations. Scientific Reports, 2020, 10, 13587.	1.6	8
45	Human Î±B-crystallin discriminates between aggregation-prone and function-preserving variants of a client protein. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129502.	1.1	7
46	Specific ion interactions with aromatic rings in aqueous solutions: Comparison of molecular dynamics simulations with a thermodynamic solute partitioning model and Raman spectroscopy. Chemical Physics Letters, 2015, 638, 1-8.	1.2	6
47	Role of Conformational Flexibility in Monte Carlo Simulations of Many-Protein Systems. Journal of Chemical Theory and Computation, 2019, 15, 1399-1408.	2.3	6
48	Thermodynamics and Mechanism of the Membrane Permeation of Hv1 Channel Blockers. Journal of Membrane Biology, 2021, 254, 5-16.	1.0	6
49	Gating energetics of a voltageâ€dependent K⁺ channel pore domain. Journal of Computational Chemistry, 2017, 38, 1472-1478.	1.5	4
50	Effects of Cardiolipin on the Conformational Dynamics of Membrane-Anchored Bcl-xL. International Journal of Molecular Sciences, 2021, 22, 9388.	1.8	4
51	Voltage-Dependent Profile Structures of a Kv-Channel via Time-Resolved Neutron Interferometry. Biophysical Journal, 2019, 117, 751-766.	0.2	3
52	Structure of a DOTAP Lipid Bilayer: A Concerted Neutron Scattering and Molecular Dynamics Study. Biophysical Journal, 2010, 98, 492a.	0.2	1
53	Down-State Model of the KvAP Full Channel. Biophysical Journal, 2010, 98, 315a.	0.2	1
54	Atomistic Molecular Dynamics Simulations of Drosophila Orai in a Hydrated Lipid Bilayer. Biophysical Journal, 2014, 106, 316a.	0.2	1

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55	Anomalous Diffusion of Peripheral Membrane Signaling Proteins from All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 9990-9998.	1.2	1
56	Down-State Model of the KvAP Voltage-Sensing Domain. Biophysical Journal, 2009, 96, 484a.	0.2	0
57	Neutron Scattering and MD Simulation Study of DOPC and DOPC/cholesterol Bilayers. Biophysical Journal, 2010, 98, 493a.	0.2	0
58	A potassium Channel Voltage-Sensing Domain in a Non-Phospholipid Bilayer. Biophysical Journal, 2011, 100, 282a.	0.2	0
59	Proton Conduction via Water Wire in the Hv1 Proton Channel. Biophysical Journal, 2011, 100, 131a.	0.2	0
60	Voltage-Gating in the Hv1 Proton Channel: Clues from Atomistic Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 686a.	0.2	0
61	Microscopic Origin of Gating Current Fluctuations in a Potassium Channel Voltage Sensor. Biophysical Journal, 2012, 102, 686a.	0.2	0
62	Molecular Dynamics Simulation Studies of Ion Permeation Pathways and Energetics in the Hv1 Proton Channel. Biophysical Journal, 2013, 104, 276a.	0.2	0
63	Molecular Dynamics Simulations of Gammas-Crystallin. Biophysical Journal, 2013, 104, 46a.	0.2	0
64	Atomistic Modeling of Ion Conduction through Voltage-Sensing Domains. Biophysical Journal, 2014, 106, 538a.	0.2	0
65	Introducing Molecular Flexibility in Efficient Simulations of Many-Protein Systems. Biophysical Journal, 2015, 108, 470a.	0.2	0
66	Multi-Microsecond Molecular Dynamics Simulations of the HV1 Proton Channel. Biophysical Journal, 2016, 110, 282a-283a.	0.2	0
67	An Arginine-Rich Loop is Critical for the Modulation of the Water Permeability of Aquaporin 0. Biophysical Journal, 2016, 110, 382a-383a.	0.2	0
68	Modeling Interprotein Interactions in Concentrated Solutions of Wild-Type and Cataract-Related Variants of Î³D- and Î³S-Crystallins. Biophysical Journal, 2016, 110, 386a.	0.2	0
69	Computational Study of Anthracycline Interactions with Membrane-Embedded P-Glycoprotein. Biophysical Journal, 2016, 110, 57a.	0.2	0
70	Computational Insights on Small Molecule Binding to the Hv1 Proton Channel. Biophysical Journal, 2019, 116, 432a.	0.2	0