Giacomo Fiorin

List of Publications by Year
in descending order

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38 papers	4,446 citations	304743 22 h-index	330143 37 g-index
41 all docs	41 docs citations	41 times ranked	5458 citing authors

#	Article	IF	Citations
1	Human Learning for Molecular Simulations: The Collective Variables Dashboard in VMD. Journal of Chemical Theory and Computation, 2022, 18, 1945-1956.	5.3	8
2	SPICA Force Field for Proteins and Peptides. Journal of Chemical Theory and Computation, 2022, 18, 3204-3217.	5.3	21
3	Bringing discrete-time Langevin splitting methods into agreement with thermodynamics. Journal of Chemical Physics, 2021, 155, 184104.	3.0	3
4	Direct Derivation of Free Energies of Membrane Deformation and Other Solvent Density Variations From Enhanced Sampling Molecular Dynamics. Journal of Computational Chemistry, 2020, 41, 449-459.	3.3	26
5	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
6	The challenge of stochastic StÃ¸rmerâ€“Verlet thermostats generating correct statistics. Journal of Chemical Physics, 2020, 153, 134101.	3.0	5
7	Data-guided Multi-Map variables for ensemble refinement of molecular movies. Journal of Chemical Physics, 2020, 153, 214102.	3.0	12
8	Coexistence of Lipid Phases Stabilizes Interstitial Water in the Outer Layer of Mammalian Skin. Biophysical Journal, 2020, 118, 1588-1601.	0.5	13
9	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq1 1 0.784314 rgBT /Overl	2.4	7
10	Structural Characterization of Biomolecules through Atomistic Simulations Guided by DEER Measurements. Structure, 2019, 27, 359-370.e12.	3.3	20
11	Aggregation of poly(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 347 Td (xmlns:mml="http://www.w3.org/1998/Math/M	2.4	5
12	Large-scale state-dependent membrane remodeling by a transporter protein. ELife, 2019, 8, .	6.0	42
13	Mechanically Strong Polymer Sheets from Aligned Ultrahigh-Molecular-Weight Polyethylene Nanocomposites. Journal of Physical Chemistry Letters, 2018, 9, 2652-2658.	4.6	6
14	Infrared and fluorescence assessment of the hydration status of the tryptophan gate in the influenza A M2 proton channel. Physical Chemistry Chemical Physics, 2016, 18, 28939-28950.	2.8	19
15	Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes. Journal of Chemical Physics, 2015, 143, 243144.	3.0	55
16	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	3.2	26
17	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14260-14265.	7.1	92
18	Hydrogen-Bonded Water Molecules in the M2 Channel of the Influenza A Virus Guide the Binding Preferences of Ammonium-Based Inhibitors. Journal of Physical Chemistry B, 2015, 119, 1173-1183.	2.6	33

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19	Dehydration of multilamellar fatty acid membranes: Towards a computational model of the stratum corneum. Journal of Chemical Physics, 2014, 141, 22D526.	3.0	9
20	Flipping in the Pore: Discovery of Dual Inhibitors That Bind in Different Orientations to the Wild-Type versus the Amantadine-Resistant S31N Mutant of the Influenza A Virus M2 Proton Channel. Journal of the American Chemical Society, 2014, 136, 17987-17995.	13.7	78
21	Supramolecular Polymerization of Benzene-1,3,5-tricarboxamide: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 5218-5228.	2.6	61
22	Binding of the Antitubercular Pro-Drug Isoniazid in the Heme Access Channel of Catalase-Peroxidase (KatG). A Combined Structural and Metadynamics Investigation. Journal of Physical Chemistry B, 2014, 118, 2924-2931.	2.6	27
23	Structure of Water at Charged Interfaces: A Molecular Dynamics Study. Langmuir, 2014, 30, 8056-8065.	3.5	130
24	Exploring Histidine Conformations in the M2 Channel Lumen of the Influenza A Virus at Neutral pH via Molecular Simulations. Journal of Physical Chemistry Letters, 2013, 4, 3067-3071.	4.6	14
25	Using collective variables to drive molecular dynamics simulations. Molecular Physics, 2013, 111, 3345-3362.	1.7	750
26	Asp44 Stabilizes the Trp41 Gate of the M2 Proton Channel of Influenza A Virus. Structure, 2013, 21, 2033-2041.	3.3	34
27	Structure and inhibition of the drug-resistant S31N mutant of the M2 ion channel of influenza A virus. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1315-1320.	7.1	204
28	Discovery of Novel Dual Inhibitors of the Wild-Type and the Most Prevalent Drug-Resistant Mutant, S31N, of the M2 Proton Channel from Influenza A Virus. Journal of Medicinal Chemistry, 2013, 56, 2804-2812.	6.4	88
29	Pore waters regulate ion permeation in a calcium release-activated calcium channel. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17332-17337.	7.1	65
30	Molecular Dynamics Simulation Directed Rational Design of Inhibitors Targeting Drug-Resistant Mutants of Influenza A Virus M2. Journal of the American Chemical Society, 2011, 133, 12834-12841.	13.7	127
31	Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3958-3963.	7.1	65
32	The Flu's Proton Escort. Science, 2010, 330, 456-458.	12.6	11
33	Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15075-15080.	7.1	243
34	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. Journal of Chemical Theory and Computation, 2010, 6, 35-47.	5.3	366
35	Multiple Proton Confinement in the M2 Channel from the Influenza A Virus. Journal of Physical Chemistry C, 2010, 114, 20856-20863.	3.1	31
36	Functional Studies and Modeling of Pore-Lining Residue Mutants of the Influenza A Virus M2 Ion Channel. Biochemistry, 2010, 49, 696-708.	2.5	107

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37	On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation. Journal of Physical Chemistry B, 2010, 114, 5161-5169.	2.6	89
38	Shear response in crystalline models of poly(p-phenylene terephthalamide). Molecular Physics, 0, , e1948122.	1.7	3