Luca Monticelli

List of Publications by Year
in descending order

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Version: 2024-02-01

87 papers	8,321 citations	81434 41 h-index	68831 81 g-index
90 all docs	90 docs citations	90 times ranked	10168 citing authors

#	Article	IF	Citations
1	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	58
2	Polystyrene perturbs the structure, dynamics, and mechanical properties of DPPC membranes: An experimental and computational study. Journal of Colloid and Interface Science, 2022, 605, 110-119.	5.0	15
3	Polyply; a python suite for facilitating simulations of macromolecules and nanomaterials. Nature Communications, 2022, 13, 68.	5.8	48
4	Substrate-bound and substrate-free outward-facing structures of a multidrug ABC exporter. Science Advances, 2022, 8, eabg9215.	4.7	27
5	Interaction of Phthalates with Lipid Bilayer Membranes. Journal of Physical Chemistry B, 2022, 126, 4679-4688.	1.2	3
6	Elastic moduli of lipid membranes: Reproducibility of AFM measures. Chemistry and Physics of Lipids, 2021, 234, 105011.	1.5	15
7	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. Frontiers in Molecular Biosciences, 2021, 8, 657222.	1.6	25
8	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
9	Effect of quercetin on lipid membrane rigidity: assessment by atomic force microscopy and molecular dynamics simulations. BBA Advances, 2021, 1, 100018.	0.7	10
10	Triacylglycerols sequester monotopic membrane proteins to lipid droplets. Nature Communications, 2020, 11, 3944.	5.8	46
11	Understanding the Functional Properties of Lipid Heterogeneity in Pulmonary Surfactant Monolayers at the Atomistic Level. Frontiers in Cell and Developmental Biology, 2020, 8, 581016.	1.8	18
12	On Calculating the Bending Modulus of Lipid Bilayer Membranes from Buckling Simulations. Journal of Physical Chemistry B, 2020, 124, 6299-6311.	1.2	42
13	Size-dependent aggregation of hydrophobic nanoparticles in lipid membranes. Nanoscale, 2020, 12, 9452-9461.	2.8	13
14	Role of Ligand Conformation on Nanoparticleâ€“Protein Interactions. Journal of Physical Chemistry B, 2019, 123, 1764-1769.	1.2	23
15	Membrane Asymmetry Imposes Directionality on Lipid Droplet Emergence from the ER. Developmental Cell, 2019, 50, 25-42.e7.	3.1	114
16	To Bud or Not to Bud: A Perspective on Molecular Simulations of Lipid Droplet Budding. Frontiers in Molecular Biosciences, 2019, 6, 124.	1.6	27
17	Transferable MARTINI Model of Poly(ethylene Oxide). Journal of Physical Chemistry B, 2018, 122, 7436-7449.	1.2	99
18	Molecular Dynamics Simulations. , 2018, , 1-7.		0

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19	Quantification of Detergents Complexed with Membrane Proteins. Scientific Reports, 2017, 7, 41751.	1.6	66
20	On Atomistic Models for Molecular Oxygen. Journal of Physical Chemistry B, 2017, 121, 518-528.	1.2	19
21	Interaction of hydrophobic polymers with model lipid bilayers. Scientific Reports, 2017, 7, 6357.	1.6	56
22	Molecular electrometer and binding of cations to phospholipid bilayers. Physical Chemistry Chemical Physics, 2016, 18, 32560-32569.	1.3	78
23	Gold nanoparticles in model biological membranes: A computational perspective. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2380-2389.	1.4	67
24	The Membrane Bending Modulus in Experiments and Simulations. Advances in Biomembranes and Lipid Self-Assembly, 2016, , 117-143.	0.3	24
25	The C-terminal Domains of Apoptotic BH3-only Proteins Mediate Their Insertion into Distinct Biological Membranes. Journal of Biological Chemistry, 2016, 291, 25207-25216.	1.6	14
26	Simulating the interaction of lipid membranes with polymer and ligand-coated nanoparticles. Advances in Physics: X, 2016, 1, 276-296.	1.5	21
27	Initiating Polyglutamine Aggregation --- Computational Clarification of the Structural Details. Biophysical Journal, 2015, 108, 386a.	0.2	0
28	Open Collaboration that uses NMR Data to Judge the Correctness of Phospholipid Glycerol and Head Group Structures in Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 411a.	0.2	0
29	Calculating the free energy of transfer of small solutes into a model lipid membrane: Comparison between metadynamics and umbrella sampling. Journal of Chemical Physics, 2015, 143, 144108.	1.2	57
30	MARTINI Coarse-Grained Models of Polyethylene and Polypropylene. Journal of Physical Chemistry B, 2015, 119, 8209-8216.	1.2	82
31	Lipid monolayer disruption caused by aggregated carbon nanoparticles. RSC Advances, 2015, 5, 11676-11685.	1.7	47
32	C 60 fullerene promotes lung monolayer collapse. Journal of the Royal Society Interface, 2015, 12, 20140931.	1.5	31
33	Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions. Journal of Physical Chemistry B, 2015, 119, 15075-15088.	1.2	109
34	Coarse-Grained Force Fields for Molecular Simulations. Methods in Molecular Biology, 2015, 1215, 125-149.	0.4	18
35	Hydrophobic Compounds Reshape Membrane Domains. PLoS Computational Biology, 2014, 10, e1003873.	1.5	58
36	Modeling the effect of nano-sized polymer particles on the properties of lipid membranes. Journal of Physics Condensed Matter, 2014, 26, 503101.	0.7	34

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37	Lipid Membranes as Solvents for Carbon Nanoparticles. Physical Review Letters, 2014, 112, 068102.	2.9	61
38	Plasticity and conformational equilibria of influenza fusion peptides in model lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1169-1179.	1.4	10
39	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. Soft Matter, 2014, 10, 3716.	1.2	84
40	Stable Polyglutamine Dimers Can Contain Î²-Hairpins with Interdigitated Side Chainsâ€"But Not Î±-Helices, Î²-Nanotubes, Î²-Pseudohelices, or Steric Zippers. Biophysical Journal, 2014, 106, 1721-1728.	0.2	9
41	Polystyrene Nanoparticles Perturb Lipid Membranes. Journal of Physical Chemistry Letters, 2014, 5, 241-246.	2.1	266
42	Lipid Membranes as Solvent for Carbon Nanoparticles. Biophysical Journal, 2014, 106, 290a.	0.2	0
43	Partitioning and solubility of C₆₀fullerene in lipid membranes. Physica Scripta, 2013, 87, 058503.	1.2	21
44	Interaction of Pristine and Functionalized Carbon Nanotubes with Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 12113-12123.	1.2	66
45	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. Faraday Discussions, 2013, 161, 397-417.	1.6	170
46	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. Chemistry and Physics of Lipids, 2013, 169, 95-105.	1.5	111
47	Force Fields for Classical Molecular Dynamics. Methods in Molecular Biology, 2013, 924, 197-213.	0.4	101
48	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 3282-3292.	2.3	67
49	Mechanism for translocation of fluoroquinolones across lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2563-2571.	1.4	76
50	Interaction of C70 fullerene with the Kv1.2 potassium channel. Physical Chemistry Chemical Physics, 2012, 14, 12526.	1.3	17
51	Assessing Polyglutamine Conformation in the Nucleating Event by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 10259-10265.	1.2	31
52	Mechanism of Taq DNA Polymerase Inhibition by Fullerene Derivatives: Insight from Computer Simulations. Journal of Physical Chemistry B, 2012, 116, 10676-10683.	1.2	22
53	A Coarse-Grained MARTINI Model of Polyethylene Glycol and of Polyoxyethylene Alkyl Ether Surfactants. Journal of Physical Chemistry B, 2012, 116, 14353-14362.	1.2	90
54	On Atomistic and Coarse-Grained Models for C₆₀ Fullerene. Journal of Chemical Theory and Computation, 2012, 8, 1370-1378.	2.3	127

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55	A Novel United-Atom Force Field for Phosphatidylglycerols. Biophysical Journal, 2011, 100, 150a-151a.	0.2	0
56	A MARTINI Coarse-Grained Model of a Thermoset Polyester Coating. Macromolecules, 2011, 44, 6198-6208.	2.2	66
57	Coarse-graining polymers with the MARTINI force-field: polystyrene as a benchmark case. Soft Matter, 2011, 7, 698-708.	1.2	216
58	Free Volume Theory Applied to Lateral Diffusion in Langmuir Monolayers: Atomistic Simulations for a Protein-Free Model of Lung Surfactant. Langmuir, 2010, 26, 15436-15444.	1.6	42
59	Interpretation of 2H-NMR Experiments on the Orientation of the Transmembrane Helix WALP23 by Computer Simulations. Biophysical Journal, 2010, 99, 1455-1464.	0.2	43
60	Membrane Proteins Diffuse as Dynamic Complexes with Lipids. Journal of the American Chemical Society, 2010, 132, 7574-7575.	6.6	157
61	Membrane Protein Dynamics from Femtoseconds to Seconds. Methods in Molecular Biology, 2010, 654, 423-440.	0.4	10
62	Calgary Lipids: A Lipid Force Field for Molecular Simulations. Biophysical Journal, 2010, 98, 668a.	0.2	1
63	Effects of carbon nanoparticles on lipid membranes: a molecular simulation perspective. Soft Matter, 2009, 5, 4433.	1.2	116
64	Interaction of Fullerene with Model Cell Membranes: a Computer Simulation Study. Biophysical Journal, 2009, 96, 365a-366a.	0.2	0
65	Visualization of Complex Processes in Lipid Systems Using Computer Simulations and Molecular Graphics. , 2009, 580, 317-338.		0
66	Molecular simulation of multistate peptide dynamics: A comparison between microsecond timescale sampling and multiple shorter trajectories. Journal of Computational Chemistry, 2008, 29, 1740-1752.	1.5	48
67	Computer simulation study of fullerene translocation through lipid membranes. Nature Nanotechnology, 2008, 3, 363-368.	15.6	459
68	The MARTINI Coarse-Grained Force Field: Extension to Proteins. Journal of Chemical Theory and Computation, 2008, 4, 819-834.	2.3	2,178
69	The molecular mechanism of lipid monolayer collapse. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10803-10808.	3.3	245
70	Pressureâ˜Area Isotherm of a Lipid Monolayer from Molecular Dynamics Simulations. Langmuir, 2007, 23, 12617-12623.	1.6	161
71	An Elevated Level of Cholesterol Impairs Self-Assembly of Pulmonary Surfactant into a Functional Film. Biophysical Journal, 2007, 93, 674-683.	0.2	89
72	Effect of Lipid Peroxidation on the Properties of Lipid Bilayers: A Molecular Dynamics Study. Biophysical Journal, 2007, 93, 4225-4236.	0.2	502

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73	The Molecular Mechanism of Monolayer-Bilayer Transformations of Lung Surfactant from Molecular Dynamics Simulations. Biophysical Journal, 2007, 93, 3775-3782.	0.2	97
74	Membrane protein simulations with a united-atom lipid and all-atom protein model: lipidâ€“protein interactions, side chain transfer free energies and model proteins. Journal of Physics Condensed Matter, 2006, 18, S1221-S1234.	0.7	148
75	Structural investigation of syringomycin-E using molecular dynamics simulation and NMR. European Biophysics Journal, 2006, 35, 459-467.	1.2	4
76	Assessing the influence of electrostatic schemes on molecular dynamics simulations of secondary structure forming peptides. Journal of Physics Condensed Matter, 2006, 18, S329-S345.	0.7	20
77	Folding and Mis-Folding of Peptides and Proteins: Insights from Molecular Simulations. Mini-Reviews in Medicinal Chemistry, 2005, 5, 353-359.	1.1	7
78	Mechanism of Helix Nucleation and Propagation:Â Microscopic View from Microsecond Time Scale MD Simulations. Journal of Physical Chemistry B, 2005, 109, 20064-20067.	1.2	34
79	The influence of simulation conditions in molecular dynamics investigations of model ?-sheet peptides. Theoretical Chemistry Accounts, 2004, 112, 145.	0.5	18
80	Computer simulations of voltage-gated potassium channel KvAP. International Journal of Quantum Chemistry, 2004, 100, 1071-1078.	1.0	14
81	Computer simulation of the KvAP voltage-gated potassium channel: steered molecular dynamics of the voltage sensor. FEBS Letters, 2004, 564, 325-332.	1.3	49
82	Molecular Dynamics Simulation of a Palmitoyl-Oleoyl Phosphatidylserine Bilayer with Na+ Counterions and NaCl. Biophysical Journal, 2004, 86, 1601-1609.	0.2	173
83	Conformational Studies of a Bombolitin III-Derived Peptide Mimicking the Four-Helix Bundle Structural Motif of Proteins. Journal of the American Chemical Society, 2003, 125, 15314-15323.	6.6	5
84	Selective Ligand-induced Stabilization of Active and Desensitized Parathyroid Hormone Type 1 Receptor Conformations. Journal of Biological Chemistry, 2002, 277, 38524-38530.	1.6	91
85	Molecular characterization of a ligand-tethered parathyroid hormone receptor. Biophysical Chemistry, 2002, 95, 165-172.	1.5	28
86	Interaction of bombolitin II with a membrane-mimetic environment: an NMR and molecular dynamics simulation approach. Biophysical Chemistry, 2002, 101-102, 577-591.	1.5	12
87	Determination of solution conformations of PrP106-126, a neurotoxic fragment of prion protein, by1H NMR and restrained molecular dynamics. FEBS Journal, 1999, 266, 1192-1201.	0.2	32