Luca Monticelli

List of Publications by Year
in descending order

87	8,321	71102	60623
papers	citations	41 h-index	81 g-index

90	90	90	8996
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The MARTINI Coarse-Grained Force Field: Extension to Proteins. Journal of Chemical Theory and Computation, 2008, 4, 819-834.	5.3	2,178
2	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
3	Effect of Lipid Peroxidation on the Properties of Lipid Bilayers: A Molecular Dynamics Study. Biophysical Journal, 2007, 93, 4225-4236.	0.5	502
4	Computer simulation study of fullerene translocation through lipid membranes. Nature Nanotechnology, 2008, 3, 363-368.	31.5	459
5	Polystyrene Nanoparticles Perturb Lipid Membranes. Journal of Physical Chemistry Letters, 2014, 5, 241-246.	4.6	266
6	The molecular mechanism of lipid monolayer collapse. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10803-10808.	7.1	245
7	Coarse-graining polymers with the MARTINI force-field: polystyrene as a benchmark case. Soft Matter, 2011, 7, 698-708.	2.7	216
8	Molecular Dynamics Simulation of a Palmitoyl-Oleoyl Phosphatidylserine Bilayer with Na+ Counterions and NaCl. Biophysical Journal, 2004, 86, 1601-1609.	0.5	173
9	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. Faraday Discussions, 2013, 161, 397-417.	3.2	170
10	Pressureâ˜Area Isotherm of a Lipid Monolayer from Molecular Dynamics Simulations. Langmuir, 2007, 23, 12617-12623.	3.5	161
11	Membrane Proteins Diffuse as Dynamic Complexes with Lipids. Journal of the American Chemical Society, 2010, 132, 7574-7575.	13.7	157
12	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.	1.8	148
13	On Atomistic and Coarse-Grained Models for C₆₀ Fullerene. Journal of Chemical Theory and Computation, 2012, 8, 1370-1378.	5.3	127
14	Effects of carbon nanoparticles on lipid membranes: a molecular simulation perspective. Soft Matter, 2009, 5, 4433.	2.7	116
15	Membrane Asymmetry Imposes Directionality on Lipid Droplet Emergence from the ER. Developmental Cell, 2019, 50, 25-42.e7.	7.0	114
16	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. Chemistry and Physics of Lipids, 2013, 169, 95-105.	3.2	111
17	Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions. Journal of Physical Chemistry B, 2015, 119, 15075-15088.	2.6	109
18	Force Fields for Classical Molecular Dynamics. Methods in Molecular Biology, 2013, 924, 197-213.	0.9	101

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19	Transferable MARTINI Model of Poly(ethylene Oxide). Journal of Physical Chemistry B, 2018, 122, 7436-7449.	2.6	99
20	The Molecular Mechanism of Monolayer-Bilayer Transformations of Lung Surfactant from Molecular Dynamics Simulations. Biophysical Journal, 2007, 93, 3775-3782.	0.5	97
21	Selective Ligand-induced Stabilization of Active and Desensitized Parathyroid Hormone Type 1 Receptor Conformations. Journal of Biological Chemistry, 2002, 277, 38524-38530.	3.4	91
22	A Coarse-Grained MARTINI Model of Polyethylene Glycol and of Polyoxyethylene Alkyl Ether Surfactants. Journal of Physical Chemistry B, 2012, 116, 14353-14362.	2.6	90
23	An Elevated Level of Cholesterol Impairs Self-Assembly of Pulmonary Surfactant into a Functional Film. Biophysical Journal, 2007, 93, 674-683.	0.5	89
24	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. Soft Matter, 2014, 10, 3716.	2.7	84
25	MARTINI Coarse-Grained Models of Polyethylene and Polypropylene. Journal of Physical Chemistry B, 2015, 119, 8209-8216.	2.6	82
26	Molecular electrometer and binding of cations to phospholipid bilayers. Physical Chemistry Chemical Physics, 2016, 18, 32560-32569.	2.8	78
27	Mechanism for translocation of fluoroquinolones across lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2563-2571.	2.6	76
28	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 3282-3292.	5.3	67
29	Gold nanoparticles in model biological membranes: A computational perspective. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2380-2389.	2.6	67
30	A MARTINI Coarse-Grained Model of a Thermoset Polyester Coating. Macromolecules, 2011, 44, 6198-6208.	4.8	66
31	Interaction of Pristine and Functionalized Carbon Nanotubes with Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 12113-12123.	2.6	66
32	Quantification of Detergents Complexed with Membrane Proteins. Scientific Reports, 2017, 7, 41751.	3.3	66
33	Lipid Membranes as Solvents for Carbon Nanoparticles. Physical Review Letters, 2014, 112, 068102.	7.8	61
34	Hydrophobic Compounds Reshape Membrane Domains. PLoS Computational Biology, 2014, 10, e1003873.	3.2	58
35	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	58
36	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.	3.0	57

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37	Interaction of hydrophobic polymers with model lipid bilayers. Scientific Reports, 2017, 7, 6357.	3.3	56
38	Computer simulation of the KvAP voltage-gated potassium channel: steered molecular dynamics of the voltage sensor. FEBS Letters, 2004, 564, 325-332.	2.8	49
39	Molecular simulation of multistate peptide dynamics: A comparison between microsecond timescale sampling and multiple shorter trajectories. Journal of Computational Chemistry, 2008, 29, 1740-1752.	3.3	48
40	Polyply; a python suite for facilitating simulations of macromolecules and nanomaterials. Nature Communications, 2022, 13, 68.	12.8	48
41	Lipid monolayer disruption caused by aggregated carbon nanoparticles. RSC Advances, 2015, 5, 11676-11685.	3.6	47
42	Triacylglycerols sequester monotopic membrane proteins to lipid droplets. Nature Communications, 2020, 11, 3944.	12.8	46
43	Interpretation of 2H-NMR Experiments on the Orientation of the Transmembrane Helix WALP23 by Computer Simulations. Biophysical Journal, 2010, 99, 1455-1464.	0.5	43
44	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.	3.5	42
45	On Calculating the Bending Modulus of Lipid Bilayer Membranes from Buckling Simulations. Journal of Physical Chemistry B, 2020, 124, 6299-6311.	2.6	42
46	Mechanism of Helix Nucleation and Propagation:Â Microscopic View from Microsecond Time Scale MD Simulations. Journal of Physical Chemistry B, 2005, 109, 20064-20067.	2.6	34
47	Modeling the effect of nano-sized polymer particles on the properties of lipid membranes. Journal of Physics Condensed Matter, 2014, 26, 503101.	1.8	34
48	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
49	Assessing Polyglutamine Conformation in the Nucleating Event by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 10259-10265.	2.6	31
50	C 60 fullerene promotes lung monolayer collapse. Journal of the Royal Society Interface, 2015, 12, 20140931.	3.4	31
51	Molecular characterization of a ligand-tethered parathyroid hormone receptor. Biophysical Chemistry, 2002, 95, 165-172.	2.8	28
52	To Bud or Not to Bud: A Perspective on Molecular Simulations of Lipid Droplet Budding. Frontiers in Molecular Biosciences, 2019, 6, 124.	3.5	27
53	Substrate-bound and substrate-free outward-facing structures of a multidrug ABC exporter. Science Advances, 2022, 8, eabg9215.	10.3	27
54	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. Frontiers in Molecular Biosciences, 2021, 8, 657222.	3.5	25

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55	The Membrane Bending Modulus in Experiments and Simulations. Advances in Biomembranes and Lipid Self-Assembly, 2016, , 117-143.	0.6	24
56	Role of Ligand Conformation on Nanoparticleâ€“Protein Interactions. Journal of Physical Chemistry B, 2019, 123, 1764-1769.	2.6	23
57	Mechanism of Taq DNA Polymerase Inhibition by Fullerene Derivatives: Insight from Computer Simulations. Journal of Physical Chemistry B, 2012, 116, 10676-10683.	2.6	22
58	Partitioning and solubility of C₆₀fullerene in lipid membranes. Physica Scripta, 2013, 87, 058503.	2.5	21
59	Simulating the interaction of lipid membranes with polymer and ligand-coated nanoparticles. Advances in Physics: X, 2016, 1, 276-296.	4.1	21
60	Assessing the influence of electrostatic schemes on molecular dynamics simulations of secondary structure forming peptides. Journal of Physics Condensed Matter, 2006, 18, S329-S345.	1.8	20
61	On Atomistic Models for Molecular Oxygen. Journal of Physical Chemistry B, 2017, 121, 518-528.	2.6	19
62	The influence of simulation conditions in molecular dynamics investigations of model ?-sheet peptides. Theoretical Chemistry Accounts, 2004, 112, 145.	1.4	18
63	Understanding the Functional Properties of Lipid Heterogeneity in Pulmonary Surfactant Monolayers at the Atomistic Level. Frontiers in Cell and Developmental Biology, 2020, 8, 581016.	3.7	18
64	Coarse-Grained Force Fields for Molecular Simulations. Methods in Molecular Biology, 2015, 1215, 125-149.	0.9	18
65	Interaction of C70 fullerene with the Kv1.2 potassium channel. Physical Chemistry Chemical Physics, 2012, 14, 12526.	2.8	17
66	Elastic moduli of lipid membranes: Reproducibility of AFM measures. Chemistry and Physics of Lipids, 2021, 234, 105011.	3.2	15
67	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.	9.4	15
68	Computer simulations of voltage-gated potassium channel KvAP. International Journal of Quantum Chemistry, 2004, 100, 1071-1078.	2.0	14
69	The C-terminal Domains of Apoptotic BH3-only Proteins Mediate Their Insertion into Distinct Biological Membranes. Journal of Biological Chemistry, 2016, 291, 25207-25216.	3.4	14
70	Size-dependent aggregation of hydrophobic nanoparticles in lipid membranes. Nanoscale, 2020, 12, 9452-9461.	5.6	13
71	Interaction of bombolitin II with a membrane-mimetic environment: an NMR and molecular dynamics simulation approach. Biophysical Chemistry, 2002, 101-102, 577-591.	2.8	12
72	Membrane Protein Dynamics from Femtoseconds to Seconds. Methods in Molecular Biology, 2010, 654, 423-440.	0.9	10

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73	Plasticity and conformational equilibria of influenza fusion peptides in model lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1169-1179.	2.6	10
74	Effect of quercetin on lipid membrane rigidity: assessment by atomic force microscopy and molecular dynamics simulations. BBA Advances, 2021, 1, 100018.	1.6	10
75	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.	0.5	9
76	Folding and Mis-Folding of Peptides and Proteins: Insights from Molecular Simulations. Mini-Reviews in Medicinal Chemistry, 2005, 5, 353-359.	2.4	7
77	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.	13.7	5
78	Structural investigation of syringomycin-E using molecular dynamics simulation and NMR. European Biophysics Journal, 2006, 35, 459-467.	2.2	4
79	Interaction of Phthalates with Lipid Bilayer Membranes. Journal of Physical Chemistry B, 2022, 126, 4679-4688.	2.6	3
80	Calgary Lipids: A Lipid Force Field for Molecular Simulations. Biophysical Journal, 2010, 98, 668a.	0.5	1
81	Interaction of Fullerene with Model Cell Membranes: a Computer Simulation Study. Biophysical Journal, 2009, 96, 365a-366a.	0.5	0
82	A Novel United-Atom Force Field for Phosphatidylglycerols. Biophysical Journal, 2011, 100, 150a-151a.	0.5	0
83	Lipid Membranes as Solvent for Carbon Nanoparticles. Biophysical Journal, 2014, 106, 290a.	0.5	0
84	Initiating Polyglutamine Aggregation --- Computational Clarification of the Structural Details. Biophysical Journal, 2015, 108, 386a.	0.5	0
85	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.	0.5	0
86	Visualization of Complex Processes in Lipid Systems Using Computer Simulations and Molecular Graphics. , 2009, 580, 317-338.		0
87	Molecular Dynamics Simulations. , 2018, , 1-7.		0