Siewert-Jan Marrink

List of Publications by Citations

290 papers	32,667 citations	88 h-index	177 g-index
319 ext. papers	38,101 ext. citations	7.2 avg, IF	7.57 L-index

#	Paper	IF	Citations
290	The MARTINI force field: coarse grained model for biomolecular simulations. *Journal of Physical Chemistry B*, **2007**, 111, 7812-24	3.4	3596
289	Coarse Grained Model for Semiquantitative Lipid Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 750-760	3.4	1767
288	The MARTINI Coarse-Grained Force Field: Extension to Proteins. *Journal of Chemical Theory and Computation*, **2008**, 4, 819-34	6.4	1717
287	Perspective on the Martini model. *Chemical Society Reviews*, **2013**, 42, 6801-22	58.5	805
286	Improved Parameters for the Martini Coarse-Grained Protein Force Field. *Journal of Chemical Theory and Computation*, **2013**, 9, 687-97	6.4	782
285	Simulation of water transport through a lipid membrane. *The Journal of Physical Chemistry*, **1994**, 98, 4155-4168		683
284	A computer perspective of membranes: molecular dynamics studies of lipid bilayer systems. *BBA - Biomembranes*, **1997**, 1331, 235-70		622
283	Polarizable water model for the coarse-grained MARTINI force field. *PLoS Computational Biology*, **2010**, 6, e1000810	5	587
282	Lipid organization of the plasma membrane. *Journal of the American Chemical Society*, **2014**, 136, 14554-9	16.4	519
281	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2144-55	6.4	504
280	The molecular face of lipid rafts in model membranes. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 17367-72	11.5	416
279	Combining an Elastic Network With a Coarse-Grained Molecular Force Field: Structure, Dynamics, and Intermolecular Recognition. *Journal of Chemical Theory and Computation*, **2009**, 5, 2531-43	6.4	397
278	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. *Journal of Chemical Theory and Computation*, **2014**, 10, 676-90	6.4	378
277	Antimicrobial peptides in action. *Journal of the American Chemical Society*, **2006**, 128, 12156-61	16.4	372
276	Toroidal pores formed by antimicrobial peptides show significant disorder. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 2308-17	3.8	364
275	Lipids on the move: simulations of membrane pores, domains, stalks and curves. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 149-68	3.8	363
274	Simulation of pore formation in lipid bilayers by mechanical stress and electric fields. *Journal of the American Chemical Society*, **2003**, 125, 6382-3	16.4	363

273	Permeation Process of Small Molecules across Lipid Membranes Studied by Molecular Dynamics Simulations. *The Journal of Physical Chemistry*, **1996**, 100, 16729-16738		358
272	A molecular dynamics study of the decane/water interface. *The Journal of Physical Chemistry*, **1993**, 97, 9206-9212		354
271	The power of coarse graining in biomolecular simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 225-248	7.9	346
270	Methodological Issues in Lipid Bilayer Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 9424-9433	3.4	314
269	Martini Coarse-Grained Force Field: Extension to Carbohydrates. *Journal of Chemical Theory and Computation*, **2009**, 5, 3195-210	6.4	302
268	A coarse-grained model for polyethylene oxide and polyethylene glycol: conformation and hydrodynamics. *Journal of Physical Chemistry B*, **2009**, 113, 13186-94	3.4	298
267	The mechanism of vesicle fusion as revealed by molecular dynamics simulations. *Journal of the American Chemical Society*, **2003**, 125, 11144-5	16.4	278
266	G protein-coupled receptors self-assemble in dynamics simulations of model bilayers. *Journal of the American Chemical Society*, **2007**, 129, 10126-32	16.4	275
265	Computational Modeling of Realistic Cell Membranes. *Chemical Reviews*, **2019**, 119, 6184-6226	68.1	265
264	Molecular dynamics simulation of the formation, structure, and dynamics of small phospholipid vesicles. *Journal of the American Chemical Society*, **2003**, 125, 15233-42	16.4	263
263	Simulation of gel phase formation and melting in lipid bilayers using a coarse grained model. *Chemistry and Physics of Lipids*, **2005**, 135, 223-44	3.7	261
262	Molecular dynamics simulations of hydrophilic pores in lipid bilayers. *Biophysical Journal*, **2004**, 86, 2156-64	4.9	248
261	Molecular Dynamics Simulation of the Kinetics of Spontaneous Micelle Formation. *Journal of Physical Chemistry B*, **2000**, 104, 12165-12173	3.4	248
260	Molecular dynamics simulation of a phospholipid membrane. *European Biophysics Journal*, **1994**, 22, 423-36	2.9	248
259	Effect of Undulations on Surface Tension in Simulated Bilayers. *Journal of Physical Chemistry B*, **2001**, 105, 6122-6127	3.4	237
258	The molecular mechanism of lipid monolayer collapse. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 10803-8	11.5	223
257	Simulation of the spontaneous aggregation of phospholipids into bilayers. *Journal of the American Chemical Society*, **2001**, 123, 8638-9	16.4	223
256	Molecular view of cholesterol flip-flop and chemical potential in different membrane environments. *Journal of the American Chemical Society*, **2009**, 131, 12714-20	16.4	222

255	Martini straight: Boosting performance using a shorter cutoff and GPUs. *Computer Physics Communications*, **2016**, 199, 1-7	4.2	221
254	Lipid packing drives the segregation of transmembrane helices into disordered lipid domains in model membranes. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 1343-8	11.5	193
253	Lipids out of equilibrium: energetics of desorption and pore mediated flip-flop. *Journal of the American Chemical Society*, **2006**, 128, 12462-7	16.4	187
252	Phytochemicals perturb membranes and promiscuously alter protein function. *ACS Chemical Biology*, **2014**, 9, 1788-98	4.9	184
251	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 4486-94	6.4	181
250	Dry Martini, a coarse-grained force field for lipid membrane simulations with implicit solvent. *Journal of Chemical Theory and Computation*, **2015**, 11, 260-75	6.4	181
249	Structural determinants of the supramolecular organization of G protein-coupled receptors in bilayers. *Journal of the American Chemical Society*, **2012**, 134, 10959-65	16.4	181
248	Adhesion forces of lipids in a phospholipid membrane studied by molecular dynamics simulations. *Biophysical Journal*, **1998**, 74, 931-43	2.9	181
247	Cholesterol shows preference for the interior of polyunsaturated lipid membranes. *Journal of the American Chemical Society*, **2008**, 130, 10-1	16.4	179
246	Molecular view of hexagonal phase formation in phospholipid membranes. *Biophysical Journal*, **2004**, 87, 3894-900	2.9	167
245	Computationally designed libraries for rapid enzyme stabilization. *Protein Engineering, Design and Selection*, **2014**, 27, 49-58	1.9	164
244	Emerging Diversity in Lipid-Protein Interactions. *Chemical Reviews*, **2019**, 119, 5775-5848	68.1	163
243	Enhancing Molecular n-Type Doping of Donor-Acceptor Copolymers by Tailoring Side Chains. *Advanced Materials*, **2018**, 30, 1704630	24	157
242	Efficient Algorithms for Langevin and DPD Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 3637-49	6.4	157
241	Martini Coarse-Grained Force Field: Extension to DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 3932-45	6.4	156
240	3D pressure field in lipid membranes and membrane-protein complexes. *Physical Review Letters*, **2009**, 102, 078101	7.4	156
239	Molecular dynamics simulation of a membrane/water interface: the ordering of water and its relation to the hydration force. *Langmuir*, **1993**, 9, 3122-3131	4	156
238	Mechanisms shaping cell membranes. *Current Opinion in Cell Biology*, **2014**, 29, 53-60	9	154

237	Hybrid simulations: combining atomistic and coarse-grained force fields using virtual sites. *Physical Chemistry Chemical Physics*, **2011**, 13, 10437-48	3.6	153
236	Semiconducting single-walled carbon nanotubes on demand by polymer wrapping. *Advanced Materials*, **2013**, 25, 2948-56	24	152
235	Molecular dynamics simulation of the spontaneous formation of a small DPPC vesicle in water in atomistic detail. *Journal of the American Chemical Society*, **2004**, 126, 4488-9	16.4	150
234	Molecular structure of the lecithin ripple phase. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 5392-6	11.5	146
233	Alternative mechanisms for the interaction of the cell-penetrating peptides penetratin and the TAT peptide with lipid bilayers. *Biophysical Journal*, **2009**, 97, 40-9	2.9	143
232	Curvature effects on lipid packing and dynamics in liposomes revealed by coarse grained molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2009**, 11, 2056-67	3.6	140
231	Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. *ACS Central Science*, **2018**, 4, 709-717	16.8	139
230	Pressure-area isotherm of a lipid monolayer from molecular dynamics simulations. *Langmuir*, **2007**, 23, 12617-23	4	139
229	Molecular mechanism of cyclodextrin mediated cholesterol extraction. *PLoS Computational Biology*, **2011**, 7, e1002020	5	134
228	Proton transport across transient single-file water pores in a lipid membrane studied by molecular dynamics simulations. *Biophysical Journal*, **1996**, 71, 632-47	2.9	130
227	Martini Force Field Parameters for Glycolipids. *Journal of Chemical Theory and Computation*, **2013**, 9, 1694-708	6.4	127
226	Reconstruction of atomistic details from coarse-grained structures. *Journal of Computational Chemistry*, **2010**, 31, 1333-43	3.5	127
225	Evidence for cardiolipin binding sites on the membrane-exposed surface of the cytochrome bc1. *Journal of the American Chemical Society*, **2013**, 135, 3112-20	16.4	126
224	Molecular dynamics simulations of lipid vesicle fusion in atomic detail. *Biophysical Journal*, **2007**, 92, 4254-61	4.9	125
223	Martini 3: a general purpose force field for coarse-grained molecular dynamics. *Nature Methods*, **2021**, 18, 382-388	21.6	124
222	Solvent-exposed tails as prestalk transition states for membrane fusion at low hydration. *Journal of the American Chemical Society*, **2010**, 132, 6710-8	16.4	118
221	Mixing MARTINI: electrostatic coupling in hybrid atomistic-coarse-grained biomolecular simulations. *Journal of Physical Chemistry B*, **2013**, 117, 3516-30	3.4	117
220	Identification of cardiolipin binding sites on cytochrome c oxidase at the entrance of proton channels. *Scientific Reports*, **2013**, 3, 1263	4.9	112

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218	Membrane poration by antimicrobial peptides combining atomistic and coarse-grained descriptions. *Faraday Discussions*, **2010**, 144, 431-43; discussion 445-81	3.6	112
217	Hsc70-4 Deforms Membranes to Promote Synaptic Protein Turnover by Endosomal Microautophagy. *Neuron*, **2015**, 88, 735-48	13.9	111
216	Coarse-grain modelling of protein-protein interactions. *Current Opinion in Structural Biology*, **2013**, 23, 878-86	8.1	108
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214	Molecular dynamics simulation of a charged biological membrane. *Journal of Chemical Physics*, **1996**, 104, 2713-2720	3.9	105
213	The Binary Mixing Behavior of Phospholipids in a Bilayer: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2004**, 108, 2454-2463	3.4	104
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211	Simulation of domain formation in DLPC-DSPC mixed bilayers. *Langmuir*, **2004**, 20, 7686-93	4	100
210	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. *Journal of the American Chemical Society*, **2017**, 139, 3697-3705	16.4	99
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205	Lipid-mediated interactions tune the association of glycophorin A helix and its disruptive mutants in membranes. *Physical Chemistry Chemical Physics*, **2010**, 12, 12987-96	3.6	93
204	Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models. *ChemPhysChem*, **2007**, 8, 452-61	3.2	92
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202	Enantioselective enzymes by computational design and in silico screening. *Angewandte Chemie - International Edition*, **2015**, 54, 3726-30	16.4	88

201	Pitfalls of the Martini Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 5448-5460	6.4	87
200	Computational microscopy of cyclodextrin mediated cholesterol extraction from lipid model membranes. *Scientific Reports*, **2013**, 3, 2071	4.9	84
199	Areas of monounsaturated diacylphosphatidylcholines. *Biophysical Journal*, **2009**, 97, 1926-32	2.9	84
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191	The Martini coarse-grained force field. *Methods in Molecular Biology*, **2013**, 924, 533-65	1.4	79
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178	Gaussian curvature elasticity determined from global shape transformations and local stress distributions: a comparative study using the MARTINI model. *Faraday Discussions*, **2013**, 161, 365-82; discussion 419-59	3.6	68
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173	Molecular view on protein sorting into liquid-ordered membrane domains mediated by gangliosides and lipid anchors. *Faraday Discussions*, **2013**, 161, 347-63; discussion 419-59	3.6	63
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171	Transferable MARTINI Model of Poly(ethylene Oxide). *Journal of Physical Chemistry B*, **2018**, 122, 7436-7449	3.4	62
170	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 3262-3275	3.4	60
169	Comment on "On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models" by M. Winger, D. Trzesniak, R. Baron and W. F. van Gunsteren, Phys. Chem. Chem. Phys., 2009, 11, 1934. *Physical Chemistry Chemical Physics*, **2010**, 12, 2254-6; author reply 2257-8	3.6	60
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149	Dimerization of Amino Acid Side Chains: Lessons from the Comparison of Different Force Fields. *Journal of Chemical Theory and Computation*, **2012**, 8, 1003-14	6.4	49
148	Simulation studies of pore and domain formation in a phospholipid monolayer. *Journal of Chemical Physics*, **2005**, 122, 024704	3.9	48

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146	Lateral pressure profiles in lipid monolayers. *Faraday Discussions*, **2010**, 144, 393-409; discussion 445-81	3.6	46
145	Molecular Mechanism of Lipid Nanodisk Formation by Styrene-Maleic Acid Copolymers. *Biophysical Journal*, **2018**, 115, 494-502	2.9	45
144	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 3282-92	6.4	45
143	Protein shape change has a major effect on the gating energy of a mechanosensitive channel. *Biophysical Journal*, **2011**, 100, 1651-9	2.9	45
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136	Hydrophobic compounds reshape membrane domains. *PLoS Computational Biology*, **2014**, 10, e1003873	5	42
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130	Structural investigation of MscL gating using experimental data and coarse grained MD simulations. *PLoS Computational Biology*, **2012**, 8, e1002683	5	37

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123	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. *Journal of Physical Chemistry Letters*, **2011**, 2, 2385-2390	6.4	34
122	Computationally efficient and accurate enantioselectivity modeling by clusters of molecular dynamics simulations. *Journal of Chemical Information and Modeling*, **2014**, 54, 2079-92	6.1	33
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120	Energetics Underlying Twist Polymorphisms in Amyloid Fibrils. *Journal of Physical Chemistry B*, **2018**, 122, 1081-1091	3.4	31
119	Location, tilt, and binding: a molecular dynamics study of voltage-sensitive dyes in biomembranes. *Journal of Physical Chemistry B*, **2009**, 113, 15807-19	3.4	31
118	Structural and Spectroscopic Properties of Assemblies of Self-Replicating Peptide Macrocycles. *ACS Nano*, **2017**, 11, 7858-7868	16.7	30
117	MARTINI Model for Physisorption of Organic Molecules on Graphite. *Journal of Physical Chemistry C*, **2013**, 117, 15623-15631	3.8	30
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115	The freezing process of small lipid vesicles at molecular resolution. *Soft Matter*, **2009**, 5, 4531	3.6	29
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112	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. *Journal of Physical Chemistry Letters*, **2018**, 9, 5527-5533	6.4	28

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110	Adaptive Resolution Simulation of Supramolecular Water: The Concurrent Making, Breaking, and Remaking of Water Bundles. *Journal of Chemical Theory and Computation*, **2016**, 12, 4138-45	6.4	26
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