Hector Martinez-Seara

List of Publications by Year
in descending order

61 papers	3,312 citations	201385 27 h-index	168136 53 g-index
71 all docs	71 docs citations	71 times ranked	3794 citing authors

#	Article	IF	Citations
1	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
2	Anomalous Diffusion of Phospholipids and Cholesterols in a Lipid Bilayer and its Origins. Physical Review Letters, 2012, 109, 188103.	2.9	257
3	MEMBPLUGIN: studying membrane complexity in VMD. Bioinformatics, 2014, 30, 1478-1480.	1.8	215
4	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. Faraday Discussions, 2013, 161, 397-417.	1.6	170
5	Protein Crowding in Lipid Bilayers Gives Rise to Non-Gaussian Anomalous Lateral Diffusion of Phospholipids and Proteins. Physical Review X, 2016, 6, .	2.8	152
6	Excessive aggregation of membrane proteins in the Martini model. PLoS ONE, 2017, 12, e0187936.	1.1	147
7	Interplay of Unsaturated Phospholipids and Cholesterol in Membranes: Effect of the Double-Bond Position. Biophysical Journal, 2008, 95, 3295-3305.	0.2	132
8	Membrane cholesterol access into a G-protein-coupled receptor. Nature Communications, 2017, 8, 14505.	5.8	129
9	Cholesterol Induces Specific Spatial and Orientational Order in Cholesterol/Phospholipid Membranes. PLoS ONE, 2010, 5, e11162.	1.1	101
10	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	1.5	94
11	Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization. Journal of Physical Chemistry B, 2018, 122, 4546-4557.	1.2	90
12	Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Scientific Reports, 2016, 6, 19839.	1.6	89
13	Nanoscale Membrane Domain Formation Driven by Cholesterol. Scientific Reports, 2017, 7, 1143.	1.6	83
14	doGlycansâ€“Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS. Journal of Chemical Information and Modeling, 2017, 57, 2401-2406.	2.5	71
15	Cationic Au Nanoparticle Binding with Plasma Membrane-like Lipid Bilayers: Potential Mechanism for Spontaneous Permeation to Cells Revealed by Atomistic Simulations. Journal of Physical Chemistry C, 2014, 118, 11131-11141.	1.5	69
16	Effect of Double Bond Position on Lipid Bilayer Properties:â€‰ Insight through Atomistic Simulations. Journal of Physical Chemistry B, 2007, 111, 11162-11168.	1.2	65
17	Diffusion of Integral Membrane Proteins in Protein-Rich Membranes. Journal of Physical Chemistry Letters, 2017, 8, 4308-4313.	2.1	65
18	A practical guide to biologically relevant molecular simulations with charge scaling for electronic polarization. Journal of Chemical Physics, 2020, 153, 050901.	1.2	63

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19	Role of Cardiolipins in the Inner Mitochondrial Membrane: Insight Gained through Atom-Scale Simulations. Journal of Physical Chemistry B, 2009, 113, 3413-3422.	1.2	62
20	Influence ofcisdouble-bond parametrization on lipid membrane properties: How seemingly insignificant details in force-field change even qualitative trends. Journal of Chemical Physics, 2008, 129, 105103.	1.2	49
21	Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2852-2860.	1.4	46
22	Binding of Divalent Cations to Insulin: Capillary Electrophoresis and Molecular Simulations. Journal of Physical Chemistry B, 2018, 122, 5640-5648.	1.2	45
23	Two cations, two mechanisms: interactions of sodium and calcium with zwitterionic lipid membranes. Chemical Communications, 2017, 53, 5380-5383.	2.2	44
24	The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers. Small, 2019, 15, e1805046.	5.2	35
25	Efficient preparation and analysis of membrane and membrane protein systems. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2468-2482.	1.4	33
26	Atomistic fingerprint of hyaluronanâ€“CD44 binding. PLoS Computational Biology, 2017, 13, e1005663.	1.5	33
27	Overbinding and Qualitative and Quantitative Changes Caused by Simple Na⁺ and K⁺ Ions in Polyelectrolyte Simulations: Comparison of Force Fields with and without NBFIX and ECC Corrections. Journal of Chemical Theory and Computation, 2020, 16, 677-687.	2.3	33
28	A Ceramide-Regulated Element in the Late Endosomal Protein LAPTM4B Controls Amino Acid Transporter Interaction. ACS Central Science, 2018, 4, 548-558.	5.3	29
29	Simulation of Raman and Raman optical activity of saccharides in solution. Physical Chemistry Chemical Physics, 2020, 22, 1983-1993.	1.3	29
30	Binding of divalent cations to acetate: molecular simulations guided by Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 24014-24027.	1.3	28
31	Nonconverged Constraints Cause Artificial Temperature Gradients in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2021, 125, 9537-9546.	1.2	28
32	Effect of PEGylation on Drug Entry into Lipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 144-151.	1.2	26
33	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. PLoS Computational Biology, 2019, 15, e1007033.	1.5	25
34	Why is the sn-2 Chain of Monounsaturated Glycerophospholipids Usually Unsaturated whereas the sn-1 Chain Is Saturated? Studies of 1-Stearoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine (SOPC) and 1-Oleoyl-2-stearoyl-sn-glycero-3-phosphatidylcholine (OSPC) Membranes with and without Cholesterol. Journal of Physical Chemistry B, 2009, 113, 8347-8356.	1.2	22
35	Rapid diffusion of cholesterol along polyunsaturated membranes via deep dives. Physical Chemistry Chemical Physics, 2019, 21, 11660-11669.	1.3	21
36	Long-chain GM1 gangliosides alter transmembrane domain registration through interdigitation. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 870-878.	1.4	20

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37	What Can We Learn about Cholesterolâ€™s Transmembrane Distribution Based on Cholesterol-Induced Changes in Membrane Dipole Potential?. Journal of Physical Chemistry Letters, 2016, 7, 4585-4590.	2.1	19
38	N-Glycosylation can selectively block or foster different receptorâ€“ligand binding modes. Scientific Reports, 2021, 11, 5239.	1.6	18
39	Structure of Glycocalyx. Biophysical Journal, 2013, 104, 251a.	0.2	16
40	Haloalkenyl Imidoyl Halides as Multifacial Substrates in the Stereoselective Synthesis of Nâ€Alkenyl Compounds. Advanced Synthesis and Catalysis, 2021, 363, 3258-3266.	2.1	16
41	Rotational Diffusion of Membrane Proteins in Crowded Membranes. Journal of Physical Chemistry B, 2020, 124, 2994-3001.	1.2	13
42	Resolving the Equal Number Density Puzzle: Molecular Picture from Simulations of LiCl(aq) and NaCl(aq). Journal of Physical Chemistry B, 2021, 125, 3153-3162.	1.2	12
43	Use of Raman and Raman optical activity to extract atomistic details of saccharides in aqueous solution. PLoS Computational Biology, 2022, 18, e1009678.	1.5	12
44	Raman Optical Activity of Glucose and Sorbose in Extended Wavenumber Range. ChemPhysChem, 2020, 21, 1272-1279.	1.0	9
45	Nanoparticleâ€“Membrane Interactions: The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers (Small 23/2019). Small, 2019, 15, 1970124.	5.2	8
46	Molecular Dynamics Simulations of Lipid Bilayers: Simple Recipe of How to Do It. Methods in Molecular Biology, 2013, 924, 407-429.	0.4	6
47	Efficiently Computing NMR¹H and¹³C Chemical Shifts of Saccharides in Aqueous Environment. Journal of Chemical Theory and Computation, 2022, 18, 4373-4386.	2.3	6
48	Emerging Era of Biomolecular Membrane Simulations: Automated Physically-Justified Force Field Development and Quality-Evaluated Databanks. Journal of Physical Chemistry B, 2022, 126, 4169-4183.	1.2	6
49	Anisotropic diffusion of membrane proteins at experimental timescales. Journal of Chemical Physics, 2021, 155, 015102.	1.2	4
50	Changes in the Local Conformational States Caused by Simple Na+ and K+ Ions in Polyelectrolyte Simulations: Comparison of Seven Force Fields with and without NBFIX and ECC Corrections. Polymers, 2022, 14, 252.	2.0	4
51	Travelling waves in two-dimensional smectic-C domains. European Physical Journal E, 2006, 21, 111-116.	0.7	2
52	Obtaining 3D Atomistic Structure of Saccharides from Raman/ROA/NMR Spectroscopic Techniques. Biophysical Journal, 2020, 118, 298a.	0.2	2
53	Directionality of Light Absorption in Fluorescent Proteins. Biophysical Journal, 2020, 118, 311a.	0.2	1
54	Specific Spatial and Orientational Order in Phospholipid Membranes Induced by Cholesterol. Biophysical Journal, 2010, 98, 668a.	0.2	0

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55	Atomistic Simulations of Functional Gold Nanoparticles Au144(Sr)60 Interacting with Membranes. Biophysical Journal, 2013, 104, 664a.	0.2	0
56	Characterisation of Coexisting Liquid Phases in Mixtures of Dipalmitoylphosphatidylcholine and Cholesterol. Biophysical Journal, 2014, 106, 709a-710a.	0.2	0
57	Cell Membrane Composition Affects GPCR Aggregation. Biophysical Journal, 2014, 106, 517a-518a.	0.2	0
58	The Effect of Membrane Polyunsaturated Fatty Acids on Receptor Partitioning to Ordered Domains. Biophysical Journal, 2017, 112, 230a-231a.	0.2	0
59	Diffusion of Proteins and Lipids in Protein-Rich Membranes. Biophysical Journal, 2018, 114, 551a.	0.2	0
60	Distinct Interactions of Sodium and Calcium Cations and Neutral Phospholipid Membranes and How to Simulate Them. Biophysical Journal, 2019, 116, 90a-91a.	0.2	0
61	Benefits of the Electronic Continuum Correction in Bio-Force Fields. Biophysical Journal, 2020, 118, 558a.	0.2	0