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	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
2	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
3	Efficiently Computing NMR¹H and¹³C Chemical Shifts of Saccharides in Aqueous Environment. Journal of Chemical Theory and Computation, 2022, 18, 4373-4386.	2.3	6
4	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
5	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
6	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
7	N-Glycosylation can selectively block or foster different receptorâ€“ligand binding modes. Scientific Reports, 2021, 11, 5239.	1.6	18
8	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
9	Anisotropic diffusion of membrane proteins at experimental timescales. Journal of Chemical Physics, 2021, 155, 015102.	1.2	4
10	Nonconverged Constraints Cause Artificial Temperature Gradients in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2021, 125, 9537-9546.	1.2	28
11	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
12	Binding of divalent cations to acetate: molecular simulations guided by Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 24014-24027.	1.3	28
13	Obtaining 3D Atomistic Structure of Saccharides from Raman/ROA/NMR Spectroscopic Techniques. Biophysical Journal, 2020, 118, 298a.	0.2	2
14	A practical guide to biologically relevant molecular simulations with charge scaling for electronic polarization. Journal of Chemical Physics, 2020, 153, 050901.	1.2	63
15	Rotational Diffusion of Membrane Proteins in Crowded Membranes. Journal of Physical Chemistry B, 2020, 124, 2994-3001.	1.2	13
16	Benefits of the Electronic Continuum Correction in Bio-Force Fields. Biophysical Journal, 2020, 118, 558a.	0.2	0
17	Simulation of Raman and Raman optical activity of saccharides in solution. Physical Chemistry Chemical Physics, 2020, 22, 1983-1993.	1.3	29
18	Raman Optical Activity of Glucose and Sorbose in Extended Wavenumber Range. ChemPhysChem, 2020, 21, 1272-1279.	1.0	9

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19	Directionality of Light Absorption in Fluorescent Proteins. Biophysical Journal, 2020, 118, 311a.	0.2	1
20	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
21	Rapid diffusion of cholesterol along polyunsaturated membranes via deep dives. Physical Chemistry Chemical Physics, 2019, 21, 11660-11669.	1.3	21
22	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. PLoS Computational Biology, 2019, 15, e1007033.	1.5	25
23	The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers. Small, 2019, 15, e1805046.	5.2	35
24	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
25	Binding of Divalent Cations to Insulin: Capillary Electrophoresis and Molecular Simulations. Journal of Physical Chemistry B, 2018, 122, 5640-5648.	1.2	45
26	Diffusion of Proteins and Lipids in Protein-Rich Membranes. Biophysical Journal, 2018, 114, 551a.	0.2	0
27	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
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	Membrane cholesterol access into a G-protein-coupled receptor. Nature Communications, 2017, 8, 14505.	5.8	129
30	Long-chain GM1 gangliosides alter transmembrane domain registration through interdigitation. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 870-878.	1.4	20
31	Two cations, two mechanisms: interactions of sodium and calcium with zwitterionic lipid membranes. Chemical Communications, 2017, 53, 5380-5383.	2.2	44
32	The Effect of Membrane Polyunsaturated Fatty Acids on Receptor Partitioning to Ordered Domains. Biophysical Journal, 2017, 112, 230a-231a.	0.2	0
33	Diffusion of Integral Membrane Proteins in Protein-Rich Membranes. Journal of Physical Chemistry Letters, 2017, 8, 4308-4313.	2.1	65
34	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
35	Nanoscale Membrane Domain Formation Driven by Cholesterol. Scientific Reports, 2017, 7, 1143.	1.6	83
36	Atomistic fingerprint of hyaluronanâ€“CD44 binding. PLoS Computational Biology, 2017, 13, e1005663.	1.5	33

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37	Excessive aggregation of membrane proteins in the Martini model. PLoS ONE, 2017, 12, e0187936.	1.1	147
38	Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Scientific Reports, 2016, 6, 19839.	1.6	89
39	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
40	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
41	Efficient preparation and analysis of membrane and membrane protein systems. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2468-2482.	1.4	33
42	Effect of PEGylation on Drug Entry into Lipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 144-151.	1.2	26
43	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
44	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
45	MEMBPLUGIN: studying membrane complexity in VMD. Bioinformatics, 2014, 30, 1478-1480.	1.8	215
46	Characterisation of Coexisting Liquid Phases in Mixtures of Dipalmitoylphosphatidylcholine and Cholesterol. Biophysical Journal, 2014, 106, 709a-710a.	0.2	0
47	Cell Membrane Composition Affects GPCR Aggregation. Biophysical Journal, 2014, 106, 517a-518a.	0.2	0
48	Atomistic Simulations of Functional Gold Nanoparticles Au144(Sr)60 Interacting with Membranes. Biophysical Journal, 2013, 104, 664a.	0.2	0
49	Molecular Dynamics Simulations of Lipid Bilayers: Simple Recipe of How to Do It. Methods in Molecular Biology, 2013, 924, 407-429.	0.4	6
50	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. Faraday Discussions, 2013, 161, 397-417.	1.6	170
51	Structure of Glycocalyx. Biophysical Journal, 2013, 104, 251a.	0.2	16
52	Anomalous Diffusion of Phospholipids and Cholesterols in a Lipid Bilayer and its Origins. Physical Review Letters, 2012, 109, 188103.	2.9	257
53	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	1.5	94
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	Cholesterol Induces Specific Spatial and Orientational Order in Cholesterol/Phospholipid Membranes. PLoS ONE, 2010, 5, e11162.	1.1	101
56	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
57	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
58	Interplay of Unsaturated Phospholipids and Cholesterol in Membranes: Effect of the Double-Bond Position. Biophysical Journal, 2008, 95, 3295-3305.	0.2	132
59	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
60	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
61	Travelling waves in two-dimensional smectic-C domains. European Physical Journal E, 2006, 21, 111-116.	0.7	2