Alex H De Vries

List of Publications by Year
in descending order

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38 papers	10,605 citations	236925 25 h-index	315739 38 g-index
38 all docs	38 docs citations	38 times ranked	8398 citing authors

#	Article	IF	Citations
1	The MARTINI Force Field:â€‰ Coarse Grained Model for Biomolecular Simulations. Journal of Physical Chemistry B, 2007, 111, 7812-7824.	2.6	4,650
2	Coarse Grained Model for Semiquantitative Lipid Simulations. Journal of Physical Chemistry B, 2004, 108, 750-760.	2.6	2,027
3	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	13.7	734
4	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
5	Martini Coarse-Grained Force Field: Extension to Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 3195-3210.	5.3	363
6	Methodological Issues in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2003, 107, 9424-9433.	2.6	337
7	Dry Martini, a Coarse-Grained Force Field for Lipid Membrane Simulations with Implicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 260-275.	5.3	236
8	Martini Force Field Parameters for Glycolipids. Journal of Chemical Theory and Computation, 2013, 9, 1694-1708.	5.3	166
9	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, 4488-4489.	13.7	164
10	Molecular structure of the lecithin ripple phase. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5392-5396.	7.1	159
11	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	5.3	159
12	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. Journal of the American Chemical Society, 2017, 139, 3697-3705.	13.7	133
13	Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1319-1330.	2.6	120
14	Transferable MARTINI Model of Poly(ethylene Oxide). Journal of Physical Chemistry B, 2018, 122, 7436-7449.	2.6	99
15	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3262-3275.	2.6	81
16	Effects of bundling on the properties of the SPC water model. Theoretical Chemistry Accounts, 2010, 125, 335-344.	1.4	73
17	Martini 3 Coarseâ€Grained Force Field: Small Molecules. Advanced Theory and Simulations, 2022, 5, .	2.8	72
18	Tight cohesion between glycolipid membranes results from balanced waterâ€“headgroup interactions. Nature Communications, 2017, 8, 14899.	12.8	61

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19	Titratable Martini model for constant pH simulations. Journal of Chemical Physics, 2020, 153, 024118.	3.0	57
20	Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598.	5.3	46
21	Martini coarse-grained models of imidazolium-based ionic liquids: from nanostructural organization to liquidâ€“liquid extraction. Green Chemistry, 2020, 22, 7376-7386.	9.0	45
22	Location, Tilt, and Binding: A Molecular Dynamics Study of Voltage-Sensitive Dyes in Biomembranes. Journal of Physical Chemistry B, 2009, 113, 15807-15819.	2.6	35
23	Capturing Cholineâ€“Aromatics Cationâ^Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	5.3	35
24	Force-field dependence of the conformational properties of Î±,Ï‰-dimethoxypolyethylene glycol. Molecular Physics, 2009, 107, 1313-1321.	1.7	28
25	Resolving Donorâ€“Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains. Advanced Functional Materials, 2020, 30, 2004799.	14.9	28
26	Investigating the Structure of Aggregates of an Amphiphilic Cyanine Dye with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 5857-5867.	2.6	22
27	Dual Resolution Membrane Simulations Using Virtual Sites. Journal of Physical Chemistry B, 2020, 124, 3944-3953.	2.6	21
28	Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. Chemical Science, 2020, 11, 11514-11524.	7.4	18
29	Nucleation Mechanisms of Self-Assembled Physisorbed Monolayers on Graphite. Journal of Physical Chemistry C, 2019, 123, 17510-17520.	3.1	15
30	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. Physical Chemistry Chemical Physics, 2020, 22, 21083-21093.	2.8	14
31	Binding of quinazolinones to c-KIT G-quadruplex; an interplay between hydrogen bonding and Ï€-Ï€ stacking. Biophysical Chemistry, 2019, 253, 106220.	2.8	11
32	Capturing Membrane Phase Separation by Dual Resolution Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5876-5884.	5.3	10
33	Coupling Coarse-Grained to Fine-Grained Models via Hamiltonian Replica Exchange. Journal of Chemical Theory and Computation, 2020, 16, 5313-5322.	5.3	9
34	Modelling structural properties of cyanine dye nanotubes at coarse-grained level. Nanoscale Advances, 2022, 4, 3033-3042.	4.6	5
35	Mechanism of Ostwald Ripening in 2D Physisorbed Assemblies at Molecular Time and Length Scale by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 24380-24385.	3.1	4
36	Direct and Regioselective Diâ€Î±â€fucosylation on the Secondary Rim of Î²â€Cyclodextrin. Chemistry - A European Journal, 2019, 25, 6722-6727.	3.3	4

#	Article	IF	Citations
37	Cryogenic TEM imaging of artificial light harvesting complexes outside equilibrium. Scientific Reports, 2022, 12, 5552.	3.3	4
38	Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. Molecules, 2021, 26, 6069.	3.8	3