Alex H De Vries

List of Publications by Year
in descending order

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38 papers	10,605 citations	236612 25 h-index	315357 38 g-index
38 all docs	38 docs citations	38 times ranked	8398 citing authors

#	Article	IF	Citations
1	Cryogenic TEM imaging of artificial light harvesting complexes outside equilibrium. Scientific Reports, 2022, 12, 5552.	1.6	4
2	Martini 3 Coarseâ€Grained Force Field: Small Molecules. Advanced Theory and Simulations, 2022, 5, .	1.3	72
3	Modelling structural properties of cyanine dye nanotubes at coarse-grained level. Nanoscale Advances, 2022, 4, 3033-3042.	2.2	5
4	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
5	Capturing Membrane Phase Separation by Dual Resolution Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5876-5884.	2.3	10
6	Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. Molecules, 2021, 26, 6069.	1.7	3
7	Titratable Martini model for constant pH simulations. Journal of Chemical Physics, 2020, 153, 024118.	1.2	57
8	Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. Chemical Science, 2020, 11, 11514-11524.	3.7	18
9	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. Physical Chemistry Chemical Physics, 2020, 22, 21083-21093.	1.3	14
10	Martini coarse-grained models of imidazolium-based ionic liquids: from nanostructural organization to liquidâ€“liquid extraction. Green Chemistry, 2020, 22, 7376-7386.	4.6	45
11	Resolving Donorâ€“Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains. Advanced Functional Materials, 2020, 30, 2004799.	7.8	28
12	Coupling Coarse-Grained to Fine-Grained Models via Hamiltonian Replica Exchange. Journal of Chemical Theory and Computation, 2020, 16, 5313-5322.	2.3	9
13	Capturing Cholineâ€“Aromatics Cationâ^Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	2.3	35
14	Dual Resolution Membrane Simulations Using Virtual Sites. Journal of Physical Chemistry B, 2020, 124, 3944-3953.	1.2	21
15	Binding of quinazolinones to c-KIT G-quadruplex; an interplay between hydrogen bonding and Ï€-Ï€ stacking. Biophysical Chemistry, 2019, 253, 106220.	1.5	11
16	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	2.3	159
17	Nucleation Mechanisms of Self-Assembled Physisorbed Monolayers on Graphite. Journal of Physical Chemistry C, 2019, 123, 17510-17520.	1.5	15
18	Direct and Regioselective Diâ€Î±â€fucosylation on the Secondary Rim of Î²â€Cyclodextrin. Chemistry - A European Journal, 2019, 25, 6722-6727.	1.7	4

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19	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.	1.5	4
20	Transferable MARTINI Model of Poly(ethylene Oxide). Journal of Physical Chemistry B, 2018, 122, 7436-7449.	1.2	99
21	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. Journal of the American Chemical Society, 2017, 139, 3697-3705.	6.6	133
22	Tight cohesion between glycolipid membranes results from balanced waterâ€“headgroup interactions. Nature Communications, 2017, 8, 14899.	5.8	61
23	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3262-3275.	1.2	81
24	Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1319-1330.	1.4	120
25	Dry Martini, a Coarse-Grained Force Field for Lipid Membrane Simulations with Implicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 260-275.	2.3	236
26	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	6.6	734
27	Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598.	2.3	46
28	Investigating the Structure of Aggregates of an Amphiphilic Cyanine Dye with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 5857-5867.	1.2	22
29	Martini Force Field Parameters for Glycolipids. Journal of Chemical Theory and Computation, 2013, 9, 1694-1708.	2.3	166
30	Effects of bundling on the properties of the SPC water model. Theoretical Chemistry Accounts, 2010, 125, 335-344.	0.5	73
31	Force-field dependence of the conformational properties of Î±,Ï‰-dimethoxypolyethylene glycol. Molecular Physics, 2009, 107, 1313-1321.	0.8	28
32	Martini Coarse-Grained Force Field: Extension to Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 3195-3210.	2.3	363
33	Location, Tilt, and Binding: A Molecular Dynamics Study of Voltage-Sensitive Dyes in Biomembranes. Journal of Physical Chemistry B, 2009, 113, 15807-15819.	1.2	35
34	The MARTINI Force Field:â€‰ Coarse Grained Model for Biomolecular Simulations. Journal of Physical Chemistry B, 2007, 111, 7812-7824.	1.2	4,650
35	Molecular structure of the lecithin ripple phase. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5392-5396.	3.3	159
36	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.	6.6	164

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37	Coarse Grained Model for Semiquantitative Lipid Simulations. Journal of Physical Chemistry B, 2004, 108, 750-760.	1.2	2,027
38	Methodological Issues in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2003, 107, 9424-9433.	1.2	337