# Alex H De Vries

List of Publications by Year
in descending order

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Version: 2024-02-01

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|---|---|---|---|
| 38 papers | 10,605 citations | 236833 25 h-index | 315616 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. | 1.2 | 4,650 |
| 2 | Coarse Grained Model for Semiquantitative Lipid Simulations. Journal of Physical Chemistry B, 2004, 108, 750-760. | 1.2 | 2,027 |
| 3 | Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559. | 6.6 | 734 |
| 4 | Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388. | 9.0 | 557 |
| 5 | Martini Coarse-Grained Force Field: Extension to Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 3195-3210. | 2.3 | 363 |
| 6 | Methodological Issues in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2003, 107, 9424-9433. | 1.2 | 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. | 2.3 | 236 |
| 8 | Martini Force Field Parameters for Glycolipids. Journal of Chemical Theory and Computation, 2013, 9, 1694-1708. | 2.3 | 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. | 6.6 | 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. | 3.3 | 159 |
| 11 | Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460. | 2.3 | 159 |
| 12 | Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. Journal of the American Chemical Society, 2017, 139, 3697-3705. | 6.6 | 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. | 1.4 | 120 |
| 14 | Transferable MARTINI Model of Poly(ethylene Oxide). Journal of Physical Chemistry B, 2018, 122, 7436-7449. | 1.2 | 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. | 1.2 | 81 |
| 16 | Effects of bundling on the properties of the SPC water model. Theoretical Chemistry Accounts, 2010, 125, 335-344. | 0.5 | 73 |
| 17 | Martini 3 Coarseâ€Grained Force Field: Small Molecules. Advanced Theory and Simulations, 2022, 5, . | 1.3 | 72 |
| 18 | Tight cohesion between glycolipid membranes results from balanced waterâ€“headgroup interactions. Nature Communications, 2017, 8, 14899. | 5.8 | 61 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Titratable Martini model for constant pH simulations. Journal of Chemical Physics, 2020, 153, 024118. | 1.2 | 57 |
| 20 | Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598. | 2.3 | 46 |
| 21 | Martini coarse-grained models of imidazolium-based ionic liquids: from nanostructural organization to liquidâ€“liquid extraction. Green Chemistry, 2020, 22, 7376-7386. | 4.6 | 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. | 1.2 | 35 |
| 23 | Capturing Cholineâ€“Aromatics Cationâ^Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560. | 2.3 | 35 |
| 24 | Force-field dependence of the conformational properties of Î±,Ï‰-dimethoxypolyethylene glycol. Molecular Physics, 2009, 107, 1313-1321. | 0.8 | 28 |
| 25 | 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 |
| 26 | 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 |
| 27 | Dual Resolution Membrane Simulations Using Virtual Sites. Journal of Physical Chemistry B, 2020, 124, 3944-3953. | 1.2 | 21 |
| 28 | Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. Chemical Science, 2020, 11, 11514-11524. | 3.7 | 18 |
| 29 | Nucleation Mechanisms of Self-Assembled Physisorbed Monolayers on Graphite. Journal of Physical Chemistry C, 2019, 123, 17510-17520. | 1.5 | 15 |
| 30 | Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. Physical Chemistry Chemical Physics, 2020, 22, 21083-21093. | 1.3 | 14 |
| 31 | 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 |
| 32 | Capturing Membrane Phase Separation by Dual Resolution Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5876-5884. | 2.3 | 10 |
| 33 | Coupling Coarse-Grained to Fine-Grained Models via Hamiltonian Replica Exchange. Journal of Chemical Theory and Computation, 2020, 16, 5313-5322. | 2.3 | 9 |
| 34 | Modelling structural properties of cyanine dye nanotubes at coarse-grained level. Nanoscale Advances, 2022, 4, 3033-3042. | 2.2 | 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. | 1.5 | 4 |
| 36 | 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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| 37 | Cryogenic TEM imaging of artificial light harvesting complexes outside equilibrium. Scientific Reports, 2022, 12, 5552. | 1.6 | 4 |
| 38 | Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. Molecules, 2021, 26, 6069. | 1.7 | 3 |