David van der Spoel

List of Publications by Citations

149 papers	50,583 citations	53 h-index	166 g-index
166 ext. papers	57,086 ext. citations	6 avg, IF	7.64 L-index

#	Paper	IF	Citations
149	GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. *Journal of Chemical Theory and Computation*, **2008**, 4, 435-47	6.4	11706
148	GROMACS: fast, flexible, and free. *Journal of Computational Chemistry*, **2005**, 26, 1701-18	3.5	10273
147	GROMACS: A message-passing parallel molecular dynamics implementation. *Computer Physics Communications*, **1995**, 91, 43-56	4.2	6589
146	GROMACS 3.0: a package for molecular simulation and trajectory analysis. *Journal of Molecular Modeling*, **2001**, 7, 306-317	2	5502
145	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. *Bioinformatics*, **2013**, 29, 845-54	7.2	4786
144	Potential for biomolecular imaging with femtosecond X-ray pulses. *Nature*, **2000**, 406, 752-7	50.4	1498
143	g_wham□A Free Weighted Histogram Analysis Implementation Including Robust Error and Autocorrelation Estimates. *Journal of Chemical Theory and Computation*, **2010**, 6, 3713-3720	6.4	930
142	Femtosecond diffractive imaging with a soft-X-ray free-electron laser. *Nature Physics*, **2006**, 2, 839-843	16.2	778
141	A systematic study of water models for molecular simulation: Derivation of water models optimized for use with a reaction field. *Journal of Chemical Physics*, **1998**, 108, 10220-10230	3.9	514
140	Force Field Benchmark of Organic Liquids: Density, Enthalpy of Vaporization, Heat Capacities, Surface Tension, Isothermal Compressibility, Volumetric Expansion Coefficient, and Dielectric Constant. *Journal of Chemical Theory and Computation*, **2012**, 8, 61-74	6.4	476
139	Water Determines the Structure and Dynamics of Proteins. *Chemical Reviews*, **2016**, 116, 7673-97	68.1	437
138	A temperature predictor for parallel tempering simulations. *Physical Chemistry Chemical Physics*, **2008**, 10, 2073-7	3.6	352
137	Thermodynamics of hydrogen bonding in hydrophilic and hydrophobic media. *Journal of Physical Chemistry B*, **2006**, 110, 4393-8	3.4	323
136	Efficient docking of peptides to proteins without prior knowledge of the binding site. *Protein Science*, **2002**, 11, 1729-37	6.3	314
135	Atomic-scale visualization of inertial dynamics. *Science*, **2005**, 308, 392-5	33.3	286
134	Molecular Dynamics Simulations of Dodecylphosphocholine Micelles at Three Different Aggregate Sizes:□Micellar Structure and Chain Relaxation. *Journal of Physical Chemistry B*, **2000**, 104, 6380-6388	3.4	250
133	Dynamic properties of water/alcohol mixtures studied by computer simulation. *Journal of Chemical Physics*, **2003**, 119, 7308-7317	3.9	238

132	Blind docking of drug-sized compounds to proteins with up to a thousand residues. *FEBS Letters*, **2006**, 580, 1447-50	3.8	215
131	Clocking femtosecond X rays. *Physical Review Letters*, **2005**, 94, 114801	7.4	196
130	Scrutinizing molecular mechanics force fields on the submicrosecond timescale with NMR data. *Biophysical Journal*, **2010**, 99, 647-55	2.9	175
129	Thiamin function, metabolism, uptake, and transport. *Biochemistry*, **2014**, 53, 821-35	3.2	171
128	Atomistic simulation of ion solvation in water explains surface preference of halides. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6838-6842	11.5	171
127	The Origin of Layer Structure Artifacts in Simulations of Liquid Water. *Journal of Chemical Theory and Computation*, **2006**, 2, 1-11	6.4	164
126	Molecular Dynamics Simulations of Water with Novel Shell-Model Potentials. *Journal of Physical Chemistry B*, **2001**, 105, 2618-2626	3.4	151
125	Reproducible polypeptide folding and structure prediction using molecular dynamics simulations. *Journal of Molecular Biology*, **2005**, 354, 173-83	6.5	150
124	GROMACS molecule & liquid database. *Bioinformatics*, **2012**, 28, 752-3	7.2	140
123	Large influence of cholesterol on solute partitioning into lipid membranes. *Journal of the American Chemical Society*, **2012**, 134, 5351-61	16.4	124
122	Protein structures under electrospray conditions. *Biochemistry*, **2007**, 46, 933-45	3.2	109
121	Molecular dynamics simulations of Leu-enkephalin in water and DMSO. *Biophysical Journal*, **1997**, 72, 2032-41	2.9	99
120	Speeding up parallel GROMACS on high-latency networks. *Journal of Computational Chemistry*, **2007**, 28, 2075-84	3.5	98
119	Comparison of Implicit and Explicit Solvent Models for the Calculation of Solvation Free Energy in Organic Solvents. *Journal of Chemical Theory and Computation*, **2017**, 13, 1034-1043	6.4	96
118	Properties of Organic Liquids when Simulated with Long-Range Lennard-Jones Interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 2938-44	6.4	86
117	Protein folding kinetics and thermodynamics from atomistic simulations. *Physical Review Letters*, **2006**, 96, 238102	7.4	80
116	Molecular dynamics simulations of peptides from BPTI: a closer look at amide-aromatic interactions. *Journal of Biomolecular NMR*, **1996**, 8, 229-38	3	79
115	Chemical properties, environmental fate, and degradation of seven classes of pollutants. *Chemical Research in Toxicology*, **2014**, 27, 713-37	4	78

114	Transcription-factor binding and sliding on DNA studied using micro- and macroscopic models. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 19796-801	11.5	67
113	Deformation of helix C in the low temperature L-intermediate of bacteriorhodopsin. *Journal of Biological Chemistry*, **2004**, 279, 2147-58	5.4	66
112	Bending of the calmodulin central helix: a theoretical study. *Protein Science*, **1996**, 5, 2044-53	6.3	66
111	Proteins, lipids, and water in the gas phase. *Macromolecular Bioscience*, **2011**, 11, 50-9	5.5	65
110	Model for the dynamics of a water cluster in an x-ray free electron laser beam. *Physical Review E*, **2004**, 70, 051904	2.4	65
109	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. *Journal of Computational Chemistry*, **2015**, 36, 1473-9	3.5	60
108	On the feasibility of nanocrystal imaging using intense and ultrashort X-ray pulses. *ACS Nano*, **2011**, 5, 139-46	16.7	59
107	Fluorescence probe of Trp-cage protein conformation in solution and in gas phase. *Journal of the American Chemical Society*, **2007**, 129, 6726-35	16.4	59
106	Prediction of NC□bond cleavage frequencies in electron capture dissociation of Trp-cage dications by force-field molecular dynamics simulations. *International Journal of Mass Spectrometry*, **2006**, 248, 124-135	1.9	58
105	Brute-Force Molecular Dynamics Simulations of Villin Headpiece: Comparison with NMR Parameters. *Journal of Physical Chemistry B*, **2003**, 107, 11178-11187	3.4	58
104	Force Field Benchmark of Organic Liquids. 2. Gibbs Energy of Solvation. *Journal of Chemical Information and Modeling*, **2015**, 55, 1192-201	6.1	57
103	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models. *Journal of Chemical Information and Modeling*, **2018**, 58, 1037-1052	6.1	56
102	Insights on the solubility of CO2 in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide from the microscopic point of view. *Environmental Science & Technology*, **2013**, 47, 7421-9	10.3	55
101	Evaporation from water clusters containing singly charged ions. *Physical Chemistry Chemical Physics* , **2007**, 9, 5105-11	3.6	55
100	Temperature and structural changes of water clusters in vacuum due to evaporation. *Journal of Chemical Physics*, **2006**, 125, 154508	3.9	55
99	Time-resolved WAXS reveals accelerated conformational changes in iodoretinal-substituted proteorhodopsin. *Biophysical Journal*, **2011**, 101, 1345-53	2.9	54
98	Local partition coefficients govern solute permeability of cholesterol-containing membranes. *Biophysical Journal*, **2013**, 105, 2760-70	2.9	53
97	Virus capsid dissolution studied by microsecond molecular dynamics simulations. *PLoS Computational Biology*, **2012**, 8, e1002502	5	53

96	Potential impact of an X-ray free electron laser on structural biology. *Radiation Physics and Chemistry*, **2004**, 71, 905-916	2.5	53
95	Toward prediction of functional protein pockets using blind docking and pocket search algorithms. *Protein Science*, **2011**, 20, 880-93	6.3	50
94	Auger electron cascades in water and ice. *Chemical Physics*, **2004**, 299, 277-283	2.3	49
93	Observation of structural anisotropy and the onset of liquidlike motion during the nonthermal melting of InSb. *Physical Review Letters*, **2005**, 95, 125701	7.4	49
92	Molecular recognition in different environments: Cyclodextrin dimer formation in organic solvents. *Journal of Physical Chemistry B*, **2012**, 116, 12684-93	3.4	46
91	MemBuilder: a web-based graphical interface to build heterogeneously mixed membrane bilayers for the GROMACS biomolecular simulation program. *Bioinformatics*, **2014**, 30, 439-41	7.2	44
90	Auger-electron cascades in diamond and amorphous carbon. *Physical Review B*, **2001**, 64,	3.3	44
89	Organic molecules on the surface of water droplets--an energetic perspective. *Physical Chemistry Chemical Physics*, **2012**, 14, 9537-45	3.6	43
88	Structural stability of electrosprayed proteins: temperature and hydration effects. *Physical Chemistry Chemical Physics*, **2009**, 11, 8069-78	3.6	43
87	Thermodynamics of hydronium and hydroxide surface solvation. *Chemical Science*, **2014**, 5, 1745	9.4	42
86	A direct comparison of protein structure in the gas and solution phase: the Trp-cage. *Journal of Physical Chemistry B*, **2007**, 111, 13147-50	3.4	42
85	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. *Journal of Chemical Physics*, **2016**, 145, 114305	3.9	42
84	Hawk: the image reconstruction package for coherent X-ray diffractive imaging. *Journal of Applied Crystallography*, **2010**, 43, 1535-1539	3.8	41
83	Influence of Na+ and Mg2+ ions on RNA structures studied with molecular dynamics simulations. *Nucleic Acids Research*, **2018**, 46, 4872-4882	20.1	40
82	Deciphering solution scattering data with experimentally guided molecular dynamics simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 780-7	6.4	40
81	CO2 and O2 distribution in Rubisco suggests the small subunit functions as a CO2 reservoir. *Journal of the American Chemical Society*, **2014**, 136, 3165-71	16.4	39
80	Fullerenes toxicity and electronic properties. *Environmental Chemistry Letters*, **2013**, 11, 105-118	13.3	38
79	GROMACS: the road ahead. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 710-715	7.9	38

78	Modeling of enzyme-substrate complexes for the metalloproteases MMP-3, ADAM-9 and ADAM-10. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 551-65	4.2	37
77	Space-time evolution of electron cascades in diamond. *Physical Review B*, **2002**, 66,	3.3	36
76	The Alexandria library, a quantum-chemical database of molecular properties for force field development. *Scientific Data*, **2018**, 5, 180062	8.2	34
75	Quantification of Solvent Contribution to the Stability of Noncovalent Complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 4542-51	6.4	33
74	Mechanistic Insights into Autoinhibition of the Oncogenic Chromatin Remodeler ALC1. *Molecular Cell*, **2017**, 68, 847-859.e7	17.6	32
73	Encapsulation of myoglobin in a cetyl trimethylammonium bromide micelle in vacuo: a simulation study. *Biochemistry*, **2009**, 48, 1006-15	3.2	32
72	Insight into the structural deformations of beta-cyclodextrin caused by alcohol cosolvents and guest molecules. *Journal of Physical Chemistry B*, **2012**, 116, 3880-9	3.4	31
71	Molecular dynamics simulations of a membrane protein-micelle complex in vacuo. *Journal of the American Chemical Society*, **2009**, 131, 16606-7	16.4	31
70	Free-Energy Calculations of Ionic Hydration Consistent with the Experimental Hydration Free Energy of the Proton. *Journal of Physical Chemistry Letters*, **2017**, 8, 2705-2712	6.4	30
69	Subunit interface dynamics in hexadecameric rubisco. *Journal of Molecular Biology*, **2011**, 411, 1083-98	6.5	29
68	Probing solution- and gas-phase structures of Trp-cage cations by chiral substitution and spectroscopic techniques. *International Journal of Mass Spectrometry*, **2006**, 253, 263-273	1.9	29
67	Towards phase transferable potential functions: Methodology and application to nitrogen. *Journal of Chemical Physics*, **1995**, 103, 2272-2285	3.9	29
66	Picosecond melting of ice by an infrared laser pulse: a simulation study. *Angewandte Chemie - International Edition*, **2008**, 47, 1417-20	16.4	27
65	Cooperative Binding of Cyclodextrin Dimers to Isoflavone Analogues Elucidated by Free Energy Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 7163-7173	3.8	26
64	Generalized Born and Explicit Solvent Models for Free Energy Calculations in Organic Solvents: Cyclodextrin Dimerization. *Journal of Chemical Theory and Computation*, **2015**, 11, 5103-13	6.4	25
63	Atomistic Simulation of Protein Encapsulation in Metal-Organic Frameworks. *Journal of Physical Chemistry B*, **2016**, 120, 477-84	3.4	25
62	Phase-Transferable Force Field for Alkali Halides. *Journal of Chemical Theory and Computation*, **2018**, 14, 5933-5948	6.4	24
61	sheet structures and dimer models of the two major tyrocidines, antimicrobial peptides from Bacillus aneurinolyticus. *Biochemistry*, **2013**, 52, 7798-806	3.2	21

60	Structural variability and the incoherent addition of scattered intensities in single-particle diffraction. *Physical Review E*, **2009**, 80, 031905	2.4	20
59	Polarizable Drude Model with s-Type Gaussian or Slater Charge Density for General Molecular Mechanics Force Fields. *Journal of Chemical Theory and Computation*, **2018**, 14, 5553-5566	6.4	20
58	Screening for the Location of RNA using the Chloride Ion Distribution in Simulations of Virus Capsids. *Journal of Chemical Theory and Computation*, **2012**, 8, 2474-83	6.4	19
57	Evaluation of Generalized Born Models for Large Scale Affinity Prediction of Cyclodextrin Host-Guest Complexes. *Journal of Chemical Information and Modeling*, **2016**, 56, 2080-2092	6.1	18
56	A proposed time-resolved X-ray scattering approach to track local and global conformational changes in membrane transport proteins. *Structure*, **2008**, 16, 21-8	5.2	18
55	Molecular modeling of the RNA binding N-terminal part of cowpea chlorotic mottle virus coat protein in solution with phosphate ions. *Biophysical Journal*, **1996**, 71, 2920-32	2.9	18
54	Relationship between electronic properties and drug activity of seven quinoxaline compounds: A DFT study. *Journal of Molecular Structure*, **2015**, 1091, 196-202	3.4	17
53	Mobility-based prediction of hydration structures of protein surfaces. *Bioinformatics*, **2015**, 31, 1959-65	7.2	17
52	Impact of sludge deposition on biodiversity. *Ecotoxicology*, **2015**, 24, 1799-814	2.9	17
51	Exploration of Interfacial Hydration Networks of Target-Ligand Complexes. *Journal of Chemical Information and Modeling*, **2016**, 56, 148-58	6.1	17
50	Molten alkali halides - temperature dependence of structure, dynamics and thermodynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 18516-18524	3.6	16
49	Molecular dynamics simulations of N-terminal peptides from a nucleotide binding protein. *Proteins: Structure, Function and Bioinformatics*, **1996**, 24, 450-66	4.2	16
48	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. *ACS Omega*, **2019**, 4, 13772-13781	3.9	15
47	Solution conformations of an insect neuropeptide: crustacean cardioactive peptide (CCAP). *Peptides*, **2009**, 30, 557-64	3.8	15
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45	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. *Journal of Chemical Theory and Computation*, **2020**, 16, 3307-3315	6.4	14
44	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. *Journal of Physical Chemistry A*, **2018**, 122, 8982-8988	2.8	14
43	Statistical efficiency of methods for computing free energy of hydration. *Journal of Chemical Physics*, **2018**, 149, 144111	3.9	14

42	Anopheles gambiae, Anoga-HrTH hormone, free and bound structure--a nuclear magnetic resonance experiment. *Peptides*, **2013**, 41, 94-100	3.8	13
41	Lifting a wet glass from a table: a microscopic picture. *Langmuir*, **2006**, 22, 5666-72	4	13
40	Impact of Dispersion Coefficient on Simulations of Proteins and Organic Liquids. *Journal of Physical Chemistry B*, **2018**, 122, 8018-8027	3.4	12
39	Trajectory NG: portable, compressed, general molecular dynamics trajectories. *Journal of Molecular Modeling*, **2011**, 17, 2669-85	2	12
38	Membrane vesiculation induced by proteins of the dengue virus envelope studied by molecular dynamics simulations. *Journal of Physics Condensed Matter*, **2017**, 29, 504002	1.8	11
37	Structural studies of melting on the picosecond time scale. *Physical Chemistry Chemical Physics*, **2008**, 10, 6344-9	3.6	11
36	Direct Link between Structure, Dynamics, and Thermodynamics in Molten Salts. *Journal of Physical Chemistry C*, **2019**, 123, 25596-25602	3.8	10
35	Open conformation of adipokinetic hormone receptor from the malaria mosquito facilitates hormone binding. *Peptides*, **2011**, 32, 553-9	3.8	10
34	Systematic design of biomolecular force fields. *Current Opinion in Structural Biology*, **2021**, 67, 18-24	8.1	10
33	Systematic exploration of multiple drug binding sites. *Journal of Cheminformatics*, **2017**, 9, 65	8.6	9
32	An efficient and extensible format, library, and API for binary trajectory data from molecular simulations. *Journal of Computational Chemistry*, **2014**, 35, 260-9	3.5	9
31	Molecular dynamics simulations of peptides from the central domain of smooth muscle caldesmon. *Journal of Biomolecular Structure and Dynamics*, **2004**, 21, 555-66	3.6	9
30	Systematically improved melting point prediction: a detailed physical simulation model is required. *Chemical Communications*, **2019**, 55, 12044-12047	5.8	7
29	An Intuitively Understandable Quality Measure for Theoretical Vibrational Spectra. *Journal of Physical Chemistry Letters*, **2020**, 11, 5471-5475	6.4	7
28	Deconvoluting Protein (Un)folding Structural Ensembles Using X-Ray Scattering, Nuclear Magnetic Resonance Spectroscopy and Molecular Dynamics Simulation. *PLoS ONE*, **2015**, 10, e0125662	3.7	7
27	A density functional study of 15N chemical shielding tensors in quinolines. *Chemical Physics Letters*, **2009**, 476, 196-200	2.5	7
26	Accurate absolute free energies for ligand–protein binding based on non-equilibrium approaches. *Communications Chemistry*, **2021**, 4,	6.3	7
25	Rotational and Translational Diffusion of Proteins as a Function of Concentration. *ACS Omega*, **2019**, 4, 20654-20664	3.9	7

24	Phosphorylation-induced torsion-angle strain in the active center of HPr, detected by NMR and restrained molecular dynamics refinement. *Protein Science*, **1996**, 5, 442-6	6.3	6
23	Making Soup: Preparing and Validating Models of the Bacterial Cytoplasm for Molecular Simulation. *Journal of Chemical Information and Modeling*, **2020**, 60, 322-331	6.1	6
22	Transient isomers in the photodissociation of bromoiodomethane. *Journal of Chemical Physics*, **2018**, 148, 134307	3.9	5
21	Free energy of separation of structure II clathrate hydrate in water and a light oil. *Journal of Physical Chemistry B*, **2012**, 116, 5933-40	3.4	5
20	Binding of Pollutants to Biomolecules: A Simulation Study. *Chemical Research in Toxicology*, **2016**, 29, 1679-1688	4	5
19	Microscopic origins of conductivity in molten salts unraveled by computer simulations. *Communications Chemistry*, **2021**, 4,	6.3	5
18	Quantitative predictions from molecular simulations using explicit or implicit interactions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,e1560	7.9	4
17	Carbonyl charge solvation patterns may relate to fragmentation classes in collision-activated dissociation. *Journal of the American Society for Mass Spectrometry*, **2012**, 23, 1319-25	3.5	3
16	Probing □□C chemical shielding tensors in cryptolepine and two bromo-substituted analogs for antiplasmodial activity. *Journal of Molecular Modeling*, **2011**, 17, 3289-97	2	3
15	Role of spin state on the geometry and nuclear quadrupole resonance parameters in hemin complex. *Biophysical Chemistry*, **2008**, 134, 200-6	3.5	3
14	Interactive visualization of electron density slices. *Journal of Applied Crystallography*, **2005**, 38, 563-565	3.8	3
13	Propagation of uncertainty in physicochemical data to force field predictions. *Physical Review Research*, **2020**, 2,	3.9	2
12	Protein Folding Properties from Molecular Dynamics Simulations. *Lecture Notes in Computer Science* , **2007**, 109-115	0.9	2
11	Toward a Computational Ecotoxicity Assay. *Journal of Chemical Information and Modeling*, **2020**, 60, 3792-3803	6.1	2
10	A potential for molecular simulation of compounds with linear moieties. *Journal of Chemical Physics* , **2020**, 153, 084503	3.9	2
9	Improved GROMACS Scaling on Ethernet Switched Clusters. *Lecture Notes in Computer Science*, **2006**, 404-405	0.9	2
8	The solution conformations of amino acids from molecular dynamics simulations of Gly-X-Gly peptides: comparison with NMR parameters. *Biochemistry and Cell Biology*, **1998**, 76, 164-70	3.6	2
7	Role of Host□Guest Charge Transfer in Cyclodextrin Complexation: A Computational Study. *Journal of Physical Chemistry C*, **2019**, 123, 17745-17756	3.8	1

6	A theoretical study of repeating sequence in HRP II: a combination of molecular dynamics simulations and (17)O quadrupole coupling tensors. *Biophysical Chemistry*, **2008**, 137, 76-80	3.5	1
5	Order Parameters and Algorithmic Approaches for Detection and Demarcation of Interfaces in Hydrate-Fluid and Ice-Fluid Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 5606-15	6.4	0
4	NMR refinement and peptide folding using the GROMACS software. *Journal of Biomolecular NMR*, **2021**, 75, 143-149	3	0
3	The structure of CO and CH at the interface of a poly(urethane urea) oligomer model from the microscopic point of view. *Journal of Chemical Physics*, **2021**, 155, 044704	3.9	0
2	Unexpected Effects of Cholesterol on Membrane Permeability. *Biophysical Journal*, **2013**, 104, 192a-193a	2.9	
1	Molecular Modeling of Inhibitors at Qi and Qo Sites in Cytochrome bc1 Complex110-127		