Christian D Lorenz

List of Publications by Year
in descending order

109 papers	4,594 citations	147726 31 h-index	110317 64 g-index
122 all docs	122 docs citations	122 times ranked	5494 citing authors

#	Article	IF	Citations
1	General purpose molecular dynamics simulations fully implemented on graphics processing units. Journal of Computational Physics, 2008, 227, 5342-5359.	1.9	1,322
2	Precise determination of the bond percolation thresholds and finite-size scaling corrections for the sc, fcc, and bcc lattices. Physical Review E, 1998, 57, 230-236.	0.8	291
3	Precise determination of the critical percolation threshold for the three-dimensional â€œSwiss cheeseâ€• model using a growth algorithm. Journal of Chemical Physics, 2001, 114, 3659-3661.	1.2	182
4	Atomistic Simulations of End-Linked Poly(dimethylsiloxane) Networks:Â Structure and Relaxation. Macromolecules, 2004, 37, 3857-3864.	2.2	135
5	Simulations of Nanotribology with Realistic Probe Tip Models. Langmuir, 2008, 24, 1240-1246.	1.6	115
6	Molecular Dynamics of Ionic Transport and Electrokinetic Effects in Realistic Silica Channels. Journal of Physical Chemistry C, 2008, 112, 10222-10232.	1.5	105
7	Universality of the excess number of clusters and the crossing probability function in three-dimensional percolation. Journal of Physics A, 1998, 31, 8147-8157.	1.6	91
8	Frictional dynamics of perfluorinated self-assembled monolayers on amorphous SiO2. Tribology Letters, 2005, 19, 93-98.	1.2	79
9	Salt Permeation and Exclusion in Hydroxylated and Functionalized Silica Pores. Physical Review Letters, 2006, 96, 095504.	2.9	79
10	On the hydration of the phosphocholine headgroup in aqueous solution. Journal of Chemical Physics, 2010, 133, 145103.	1.2	76
11	The delivered dose: Applying particokinetics to in vitro investigations of nanoparticle internalization by macrophages. Journal of Controlled Release, 2012, 162, 259-266.	4.8	66
12	Role of Network Connectivity on the Mechanical Properties of Highly Cross-Linked Polymers. Macromolecules, 2004, 37, 8466-8472.	2.2	64
13	Antimicrobial Peptide Potency is Facilitated by Greater Conformational Flexibility when Binding to Gram-negative Bacterial Inner Membranes. Scientific Reports, 2016, 6, 37639.	1.6	64
14	ILC1 drive intestinal epithelial and matrix remodelling. Nature Materials, 2021, 20, 250-259.	13.3	64
15	Similarity of Percolation Thresholds on the HCP and FCC Lattices. Journal of Statistical Physics, 2000, 98, 961-970.	0.5	60
16	Targeted fluorescence lifetime probes reveal responsive organelle viscosity and membrane fluidity. PLoS ONE, 2019, 14, e0211165.	1.1	58
17	Charge inversion of divalent ionic solutions in silica channels. Physical Review E, 2007, 75, 061202.	0.8	53
18	Forces between functionalized silica nanoparticles in solution. Physical Review E, 2009, 79, 050501.	0.8	53

#	Article	IF	Citations
19	LiPyphilic: A Python Toolkit for the Analysis of Lipid Membrane Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5907-5919.	2.3	47
20	Shape-dependent universality in percolation. Physica A: Statistical Mechanics and Its Applications, 1999, 266, 17-26.	1.2	45
21	Viscosity of Nanoconfined Water between Hydroxyl Basal Surfaces of Kaolinite: Classical Simulation Results. Journal of Physical Chemistry C, 2013, 117, 6096-6104.	1.5	44
22	On the interaction of hyaluronic acid with synovial fluid lipid membranes. Physical Chemistry Chemical Physics, 2019, 21, 9845-9857.	1.3	43
23	On the Structure of Solid Lipid Nanoparticles. Small, 2019, 15, e1903156.	5.2	42
24	Engineering Chirally Blind Protein Pseudocapsids into Antibacterial Persisters. ACS Nano, 2020, 14, 1609-1622.	7.3	42
25	Water Penetration of Damaged Self-Assembled Monolayers. Langmuir, 2008, 24, 5734-5739.	1.6	38
26	On the estimation of the curvatures and bending rigidity of membrane networks via a local maximum-entropy approach. Journal of Computational Physics, 2012, 231, 528-540.	1.9	38
27	Traction and nonequilibrium phase behavior of confined sheared liquids at high pressure. Physical Review E, 2013, 88, 052406.	0.8	37
28	Tribological Properties of Alkylsilane Self-Assembled Monolayers. Langmuir, 2005, 21, 11744-11748.	1.6	36
29	Hybrid gelation processes in enzymatically gelled gelatin: impact on nanostructure, macroscopic properties and cellular response. Soft Matter, 2013, 9, 6986-6999.	1.2	35
30	Temperature control in molecular dynamic simulations of non-equilibrium processes. Journal of Physics Condensed Matter, 2010, 22, 074205.	0.7	33
31	Atomistic Simulations of Langmuir Monolayer Collapse. Langmuir, 2006, 22, 10016-10024.	1.6	32
32	Hydrogen Bonding and Binding of Polybasic Residues with Negatively Charged Mixed Lipid Monolayers. Langmuir, 2008, 24, 1654-1658.	1.6	32
33	Short-Range Interactions of Concentrated Proline in Aqueous Solution. Journal of Physical Chemistry B, 2014, 118, 14267-14277.	1.2	31
34	Frictional Dynamics of Fluorine-Terminated Alkanethiol Self-Assembled Monolayers. Langmuir, 2004, 20, 10007-10014.	1.6	30
35	Micellar crystals in solution from molecular dynamics simulations. Journal of Chemical Physics, 2008, 128, 184906.	1.2	30
36	On the solvation structure of dimethylsulfoxide/water around the phosphatidylcholine head group in solution. Journal of Chemical Physics, 2011, 135, 225105.	1.2	29

#	Article	IF	Citations
37	Water Mediation Is Essential to Nucleation of Î²â€Turn Formation in Peptide Folding Motifs. Angewandte Chemie - International Edition, 2013, 52, 13091-13095.	7.2	29
38	Modulation of Dipalmitoylphosphatidylcholine Monolayers by Dimethyl Sulfoxide. Langmuir, 2014, 30, 8803-8811.	1.6	29
39	Molecular Dynamics Simulations of the Interfacial and Structural Properties of Dimethyldodecylamine-N-Oxide Micelles. Langmuir, 2011, 27, 546-553.	1.6	28
40	Elucidating the Origin of Diastereoselectivity in a Selfâ€Replicating System: Selfishness versus Altruism. Chemistry - A European Journal, 2011, 17, 468-480.	1.7	27
41	Minor sequence modifications in temporin B cause drastic changes in antibacterial potency and selectivity by fundamentally altering membrane activity. Scientific Reports, 2019, 9, 1385.	1.6	26
42	Fracture behavior of triglyceride-based adhesives. Journal of Polymer Science, Part B: Polymer Physics, 2004, 42, 3333-3343.	2.4	25
43	Glycerol Solvates DPPC Headgroups and Localizes in the Interfacial Regions of Model Pulmonary Interfaces Altering Bilayer Structure. Langmuir, 2018, 34, 6941-6954.	1.6	25
44	Morphology of bile salts micelles and mixed micelles with lipolysis products, from scattering techniques and atomistic simulations. Journal of Colloid and Interface Science, 2021, 587, 522-537.	5.0	25
45	Ion exclusion and electrokinetic effects resulting from electro-osmotic flow of salt solutions in charged silica nanopores. Physical Chemistry Chemical Physics, 2012, 14, 5935.	1.3	24
46	Timeâ€Resolved Fluorescence Anisotropy of a Molecular Rotor Resolves Microscopic Viscosity Parameters in Complex Environments. Small, 2020, 16, e1907139.	5.2	24
47	Molecular Dynamics Simulations of Water Confined between Matched Pairs of Hydrophobic and Hydrophilic Self-Assembled Monolayers. Langmuir, 2009, 25, 4535-4542.	1.6	23
48	Nanotribology of water confined between hydrophilic alkylsilane self-assembled monolayers. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 034005.	0.8	23
49	Atomistic Description of Pressure-Driven Flow of Aqueous Salt Solutions through Charged Silica Nanopores. Journal of Physical Chemistry C, 2015, 119, 12298-12311.	1.5	23
50	Solvation and Hydration of the Ceramide Headgroup in a Non-Polar Solution. Journal of Physical Chemistry B, 2015, 119, 128-139.	1.2	23
51	Atomic scale insights into ureaâ€“peptide interactions in solution. Physical Chemistry Chemical Physics, 2016, 18, 3862-3870.	1.3	23
52	Molecular insights into the behaviour of bile salts at interfaces: a key to their role in lipid digestion. Journal of Colloid and Interface Science, 2019, 556, 266-277.	5.0	22
53	Temporin L and aurein 2.5 have identical conformations but subtly distinct membrane and antibacterial activities. Scientific Reports, 2019, 9, 10934.	1.6	22
54	On the structure of water and chloride ion interactions with a peptide backbone in solution. Physical Chemistry Chemical Physics, 2013, 15, 21023.	1.3	21

#	Article	IF	Citations
55	Applications of the generalized Langevin equation: Towards a realistic description of the baths. Physical Review B, 2015, 91, .	1.1	21
56	Nanotribology of anti-friction coatings in MEMS. Jom, 2005, 57, 55-61.	0.9	20
57	Laurdan and Di-4-ANEPPDHQ Influence the Properties of Lipid Membranes: A Classical Molecular Dynamics and Fluorescence Study. Journal of Physical Chemistry B, 2020, 124, 11419-11430.	1.2	20
58	Charge of water droplets in non-polar oils. Journal of Applied Physics, 2013, 114, .	1.1	18
59	On the nature of hydrogen bonding between the phosphatidylcholine head group and water and dimethylsulfoxide. Chemical Physics, 2013, 410, 31-36.	0.9	17
60	The effects of surface defects in a catalysis model. Surface Science, 2002, 517, 75-86.	0.8	15
61	Fracture behavior of Lennard-Jones glasses. Physical Review E, 2003, 68, 021802.	0.8	15
62	Large Scale Molecular Dynamics Simulations of Vapor Phase Lubrication for MEMS. Journal of Adhesion Science and Technology, 2010, 24, 2453-2469.	1.4	15
63	Atomistic Description of the Solubilisation of Testosterone Propionate in a Sodium Dodecyl Sulfate Micelle. Journal of Physical Chemistry B, 2014, 118, 13192-13201.	1.2	15
64	Specific effects of monovalent counterions on the structural and interfacial properties of dodecyl sulfate monolayers. Physical Chemistry Chemical Physics, 2016, 18, 30394-30406.	1.3	15
65	Probe-Tip Induced Damage in Compliant Substrates. Journal of Manufacturing Science and Engineering, Transactions of the ASME, 2010, 132, .	1.3	14
66	Nonequilibrium processes from generalized Langevin equations: Realistic nanoscale systems connected to two thermal baths. Physical Review B, 2016, 93, .	1.1	14
67	A pleurocidin analogue with greater conformational flexibility, enhanced antimicrobial potency and in vivo therapeutic efficacy. Communications Biology, 2020, 3, 697.	2.0	14
68	Effects of lipid heterogeneity on model human brain lipid membranes. Soft Matter, 2021, 17, 126-135.	1.2	14
69	PRODAN differentially influences its local environment. Physical Chemistry Chemical Physics, 2018, 20, 16060-16066.	1.3	13
70	Impact of drug aggregation on the structural and dynamic properties of Triton X-100 micelles. Nanoscale, 2022, 14, 5392-5403.	2.8	13
71	Salt Interactions in Solution Prevent Direct Association of Urea with a Peptide Backbone. Journal of Physical Chemistry B, 2017, 121, 1866-1876.	1.2	12
72	Towards optimised drug delivery: structure and composition of testosterone enanthate in sodium dodecyl sulfate monolayers. Soft Matter, 2018, 14, 3135-3150.	1.2	12

#	Article	IF	Citations
73	Unsupervised Learning Unravels the Structure of Four-Arm and Linear Block Copolymer Micelles. Macromolecules, 2021, 54, 3755-3768.	2.2	12
74	Interplay of lipid and surfactant: Impact on nanoparticle structure. Journal of Colloid and Interface Science, 2021, 597, 278-288.	5.0	12
75	Molecular Dynamics Simulation: From â€œAb Initioâ€•to â€œCoarse Grainedâ€• , 2012, , 195-238.		11
76	Quantification of fibrous spatial point patterns from single-molecule localization microscopy (SMLM) data. Bioinformatics, 2017, 33, 1703-1711.	1.8	11
77	Effects of intercalated water on the lubricity of sliding layers under load: a theoretical investigation on MoS₂. 2D Materials, 2021, 8, 035052.	2.0	11
78	Plasticity and conformational equilibria of influenza fusion peptides in model lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1169-1179.	1.4	10
79	A novel method for constructing continuous intrinsic surfaces of nanoparticles. Journal of Molecular Modeling, 2017, 23, 219.	0.8	10
80	On the hydration of DOPE in solution. Journal of Chemical Physics, 2019, 150, 115104.	1.2	10
81	Understanding the pH-Directed Self-Assembly of a Four-Arm Block Copolymer. Macromolecules, 2020, 53, 11065-11076.	2.2	10
82	Asymmetric glycerophospholipids impart distinctive biophysical properties to lipid bilayers. Biophysical Journal, 2021, 120, 1746-1754.	0.2	10
83	Comparative atomic-scale hydration of the ceramide and phosphocholine headgroup in solution and bilayer environments. Journal of Chemical Physics, 2016, 144, 225101.	1.2	9
84	Proline and Water Stabilization of a Universal Two-Step Folding Mechanism for Î²-Turn Formation in Solution. Journal of the American Chemical Society, 2018, 140, 7301-7312.	6.6	9
85	Two Coexisting Membrane Structures Are Defined by Lateral and Transbilayer Interactions between Sphingomyelin and Cholesterol. Langmuir, 2020, 36, 9786-9799.	1.6	9
86	Simulation Study of the Silicon Oxide and Water Interface. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2586-2601.	0.4	8
87	Assembly of Influenza Hemagglutinin Fusion Peptides in a Phospholipid Bilayer by Coarse-grained Computer Simulations. Frontiers in Molecular Biosciences, 2015, 2, 66.	1.6	8
88	c-number quantum generalized Langevin equation for an open system. Physical Review B, 2016, 94, .	1.1	8
89	Minor Chemistry Changes Alter Surface Hydration to Control Fibronectin Adsorption and Assembly into Nanofibrils. Advanced Theory and Simulations, 2019, 2, 1900169.	1.3	8
90	On the solvation of the phosphocholine headgroup in an aqueous propylene glycol solution. Journal of Chemical Physics, 2018, 148, 135102.	1.2	7

#	Article	IF	Citations
91	On the microscopic origin of the cryoprotective effect in lysine solutions. Physical Chemistry Chemical Physics, 2020, 22, 6919-6927.	1.3	7
92	Nanocapsule designs for antimicrobial resistance. Nanoscale, 2021, 13, 10342-10355.	2.8	7
93	Nonequilibrium generalised Langevin equation for the calculation of heat transport properties in model 1D atomic chains coupled to two 3D thermal baths. Journal of Chemical Physics, 2017, 146, 164103.	1.2	6
94	Structure and Dynamics of Nanoconfined Water Between Surfactant Monolayers. Langmuir, 2020, 36, 447-455.	1.6	6
95	Supramolecular architecture of a multi-component biomimetic lipid barrier formulation. Journal of Colloid and Interface Science, 2021, 587, 597-612.	5.0	5
96	Accurate large scale modelling of graphene oxide: Ion trapping and chaotropic potential at the interface. Carbon, 2021, 174, 266-275.	5.4	5
97	NSAID solubilisation promotes morphological transitions in Triton X-114 surfactant micelles. Journal of Molecular Liquids, 2022, 356, 119050.	2.3	5
98	Temporin B Forms Hetero-Oligomers with Temporin L, Modifies Its Membrane Activity, and Increases the Cooperativity of Its Antibacterial Pharmacodynamic Profile. Biochemistry, 2022, 61, 1029-1040.	1.2	5
99	On the hydration and conformation of cocaine in solution. Chemical Physics Letters, 2017, 676, 58-64.	1.2	4
100	The Impact of Lipid Digestion on the Dynamic and Structural Properties of Micelles. Small, 2021, 17, e2004761.	5.2	4
101	On the Structure and Flip-flop of Free Docosahexaenoic Acid in a Model Human Brain Membrane. Journal of Physical Chemistry B, 2021, 125, 8038-8047.	1.2	4
102	Excess number of percolation clusters on the surface of a sphere. Physica A: Statistical Mechanics and Its Applications, 2001, 296, 1-8.	1.2	3
103	Interaction of testosterone-based compounds with dodecyl sulphate monolayers at the airâ€“water interface. Physical Chemistry Chemical Physics, 2018, 20, 8790-8801.	1.3	2
104	Drug reformulation for a neglected disease. The NANOHAT project to develop a safer more effective sleeping sickness drug. PLoS Neglected Tropical Diseases, 2021, 15, e0009276.	1.3	2
105	Fluorescence lifetime imaging for viscosity and diffusion measurements. , 2019, , .		2
106	Nanomaterial Functionalization Modulates Hard Protein Corona Formation: Atomistic Simulations Applied to Graphitic Materials. Advanced Materials Interfaces, 2022, 9, 2101236.	1.9	2
107	On the hydration structure of the pro-drug GPG-NH2 and its derivatives. Chemical Physics Letters, 2018, 706, 228-236.	1.2	1
108	Large Scale Molecular Dynamics Simulations of Vapor Phase Lubrication for MEMS. , 2011, , 117-133.		0

#	Article	IF	Citations
109	Modelling a Bistable System Strongly Coupled to a Debye Bath: A Quasiclassical Approach Based on the Generalised Langevin Equation. Computational Methods in Science and Technology, 2017, 23, .	0.3	0