RESEARCH & PUBLICATIONS

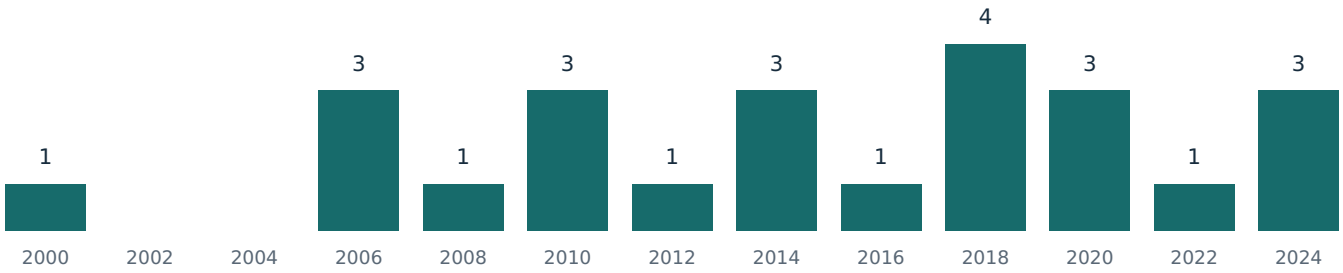
Carsten Kutzner

A publication record at a glance

25	18,542	16
ARTICLES	CITATIONS	h-INDEX

PUBLICATION ACTIVITY

Articles grouped into 2-year periods



1 articles have no publication year in the database.

MOST CITED IN THIS LIST

GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation — 15,389

2008 Journal of Chemical Theory and Computation

Tackling Exascale Software Challenges in Molecular Dynamics Simulations With GROMACS — 890

2015 Lecture Notes in Computer Science

Anatomy and Dynamics of a Supramolecular Membrane Protein Cluster — 425

2007 Science

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Ordered by publication year, newest first

2025

01 **Constant pH Simulation With FMM Electrostatics in GROMACS. (B) GPU Accelerated Hamiltonian Interpolation**
Journal of Chemical Theory and Computation · 21, 1787-1804
https://exaly.com/article/197522467
8 citations

02 **Constant pH Simulation With FMM Electrostatics in GROMACS. (A) Design and Applications**
Journal of Chemical Theory and Computation · 21, 1762-1786
https://exaly.com/article/197547752
16 citations

03 **Scaling of the GROMACS Molecular Dynamics Code to 65k CPU Cores on an HPC Cluster**
Journal of Computational Chemistry · 46, e70059
https://exaly.com/article/198528915
11 citations

2022

04 **GROMACS in the Cloud: A Global Supercomputer to Speed Up Alchemical Drug Design**
Journal of Chemical Information and Modeling · 62, 1691-1711
https://exaly.com/article/134797001
116 citations

2021

05 **A CUDA Fast Multipole Method With Highly Efficient M2L Far Field Evaluation**
International Journal of High Performance Computing Applications · 35, 97-117
https://exaly.com/article/77883740
7 citations

2020

06 **A GPU-Accelerated Fast Multipole Method for GROMACS: Performance and Accuracy**
Journal of Chemical Theory and Computation · 16, 6938-6949
https://exaly.com/article/75485839
159 citations

07 **GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation**
Lecture Notes in Computational Science and Engineering
https://exaly.com/article/83539978
4 citations

2019

08 **More Bang for Your Buck: Improved Use of GPU Nodes for GROMACS 2018**
Journal of Computational Chemistry · 40, 2418-2431
https://exaly.com/article/72209296
382 citations

Ordered by publication year, newest first

2019 / continued

09 **GROmaps: A GROMACS-Based Toolset to Analyze Density Maps Derived From Molecular Dynamics Simulations** — 89 citations

Biophysical Journal · 116, 4-11

https://exaly.com/article/74537384

10 **Automated cryo-EM structure refinement using correlation-driven molecular dynamics.** — 81 citations

ELife

https://exaly.com/article/90728357

11 **Author response: Automated cryo-EM structure refinement using correlation-driven molecular dynamics** — 1 citations

Journal unavailable

https://exaly.com/article/115485705

2016

12 **Insights Into the Function of Ion Channels by Computational Electrophysiology Simulations** — 72 citations

Biochimica Et Biophysica Acta - Biomembranes · 1858, 1741-1752

https://exaly.com/article/63878612

2015

13 **Best Bang for Your Buck: GPU Nodes for GROMACS Biomolecular Simulations** — 256 citations

Journal of Computational Chemistry · 36, 1990-2008

https://exaly.com/article/60214892

14 **Tackling Exascale Software Challenges in Molecular Dynamics Simulations With GROMACS** — 890 citations

Lecture Notes in Computer Science

https://exaly.com/article/61242563

2014

15 **Scaling of the GROMACS 4.6 Molecular Dynamics Code on SuperMUC** — 4 citations

Advances in Parallel Computing

https://exaly.com/article/135724348

2012

16 **Molecular Dynamics in Principal Component Space** — 22 citations

Journal of Physical Chemistry B · 116, 8350-4

https://exaly.com/article/54322847

Ordered by publication year, newest first

2011

17 **Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail**
218 citations
Biophysical Journal · 101, 809-817
https://exaly.com/article/50075807

18 **Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations With GROMACS**
55 citations
Journal of Chemical Theory and Computation · 7, 1381-1393
https://exaly.com/article/50390197

19 **Caught in the Act: Visualization of SNARE-Mediated Fusion Events in Molecular Detail**
144 citations
ChemBioChem · 12, 1049-1055
https://exaly.com/article/51528982

2008

20 **GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation**
15,389 citations
Journal of Chemical Theory and Computation · 4, 435-47
https://exaly.com/article/43572980

2007

21 **Anatomy and Dynamics of a Supramolecular Membrane Protein Cluster**
425 citations
Science · 317, 1072-6
https://exaly.com/article/41564358

22 **Speeding Up Parallel GROMACS on High-Latency Networks**
112 citations
Journal of Computational Chemistry · 28, 2075-2084
https://exaly.com/article/42607108

2006

23 **Improved GROMACS Scaling on Ethernet Switched Clusters**
2 citations
Lecture Notes in Computer Science
https://exaly.com/article/83200068

2000

24 **Effects of Driving Mechanisms in Geodynamo Models**
79 citations
Geophysical Research Letters · 27, 29-32
https://exaly.com/article/32260750

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Year unavailable

25 Title unavailable

Journal unavailable

https://exaly.com/article/229319639

0 citations

End of list · 25 articles. Citation counts use Exaly’s peer-reviewed cohort.