

# Frauke Gräter

## List of Publications by Year in descending order

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Version: 2024-02-01

133  
papers

7,199  
citations

81743

39  
h-index

62479

80  
g-index

138  
all docs

138  
docs citations

138  
times ranked

9872  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Anatomy of a Trafficking Organelle. <i>Cell</i> , 2006, 127, 831-846.	13.5	1,985
2	Mechanoenzymatics of titin kinase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 13385-13390.	3.3	311
3	Probing the chemistry of thioredoxin catalysis with force. <i>Nature</i> , 2007, 450, 124-127.	13.7	255
4	Plasticity of an Ultrafast Interaction between Nucleoporins and Nuclear Transport Receptors. <i>Cell</i> , 2015, 163, 734-745.	13.5	255
5	Structure and mechanism of the reversible photoswitch of a fluorescent protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 13070-13074.	3.3	253
6	Mechanically Induced Titin Kinase Activation Studied by Force-Probe Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2005, 88, 790-804.	0.2	195
7	Decoupling of size and shape fluctuations in heteropolymeric sequences reconciles discrepancies in SAXS vs. FRET measurements. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E6342-E6351.	3.3	195
8	A proton relay enhances H <sub>2</sub> O <sub>2</sub> sensitivity of GAPDH to facilitate metabolic adaptation. <i>Nature Chemical Biology</i> , 2015, 11, 156-163.	3.9	184
9	von Willebrand Factor Directly Interacts With DNA From Neutrophil Extracellular Traps. <i>Arteriosclerosis, Thrombosis, and Vascular Biology</i> , 2014, 34, 1382-1389.	1.1	129
10	Shear-Induced unfolding activates von Willebrand factor A2 domain for proteolysis. <i>Journal of Thrombosis and Haemostasis</i> , 2009, 7, 2096-2105.	1.9	113
11	A New Transferable Forcefield for Simulating the Mechanics of CaCO <sub>3</sub> Crystals. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20067-20075.	1.5	112
12	Phosphatidylinositol 4,5-bisphosphate triggers activation of focal adhesion kinase by inducing clustering and conformational changes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E3177-86.	3.3	111
13	Mechanism of Focal Adhesion Kinase Mechanosensing. <i>PLoS Computational Biology</i> , 2015, 11, e1004593.	1.5	109
14	Mechanical Response of Silk Crystalline Units from Force-Distribution Analysis. <i>Biophysical Journal</i> , 2009, 96, 3997-4005.	0.2	105
15	Signatures of hydrophobic collapse in extended proteins captured with force spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 7916-7921.	3.3	99
16	Protein/Ligand Binding Free Energies Calculated with Quantum Mechanics/Molecular Mechanics. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10474-10483.	1.2	97
17	Structural and mechanistic insights into mechanoactivation of focal adhesion kinase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 6766-6774.	3.3	90
18	CONAN: A Tool to Decode Dynamical Information from Molecular Interaction Maps. <i>Biophysical Journal</i> , 2018, 114, 1267-1273.	0.2	82

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19	Autoregulation of von Willebrand factor function by a disulfide bond switch. <i>Science Advances</i> , 2018, 4, eaaq1477.	4.7	79
20	Kirkwood's "Buff Approach Rescues Overcollapse of a Disordered Protein in Canonical Protein Force Fields. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7975-7984.	1.2	70
21	How Sequence Determines Elasticity of Disordered Proteins. <i>Biophysical Journal</i> , 2010, 99, 3863-3869.	0.2	67
22	Unique amino acid signatures that are evolutionarily conserved distinguish simple-type, epidermal and hair keratins. <i>Journal of Cell Science</i> , 2011, 124, 4221-4232.	1.2	67
23	Force-Sensitive Autoinhibition of the von Willebrand Factor Is Mediated by Interdomain Interactions. <i>Biophysical Journal</i> , 2015, 108, 2312-2321.	0.2	64
24	Atomistic Evidence of How Force Dynamically Regulates Thiol/Disulfide Exchange. <i>Journal of the American Chemical Society</i> , 2010, 132, 16790-16795.	6.6	63
25	Silk Fiber Mechanics from Multiscale Force Distribution Analysis. <i>Biophysical Journal</i> , 2011, 100, 1298-1305.	0.2	63
26	Mechanical Network in Titin Immunoglobulin from Force Distribution Analysis. <i>PLoS Computational Biology</i> , 2009, 5, e1000306.	1.5	62
27	Pheromone Discrimination by the Pheromone-Binding Protein of <i>Bombyx mori</i> . <i>Structure</i> , 2006, 14, 1577-1586.	1.6	60
28	Time-resolved force distribution analysis. <i>BMC Biophysics</i> , 2013, 6, 5.	4.4	60
29	Fast-folding $\alpha$ -helices as reversible strain absorbers in the muscle protein myomesin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 14139-14144.	3.3	59
30	Protein S-Bacillithiolation Functions in Thiol Protection and Redox Regulation of the Glyceraldehyde-3-Phosphate Dehydrogenase Gap in <i>Staphylococcus aureus</i> Under Hypochlorite Stress. <i>Antioxidants and Redox Signaling</i> , 2018, 28, 410-430.	2.5	58
31	Mechanical Force Can Fine-Tune Redox Potentials of Disulfide Bonds. <i>Biophysical Journal</i> , 2012, 102, 622-629.	0.2	51
32	POSSIBLE PATHWAY(S) OF TESTOSTERONE EGRESS FROM THE ACTIVE SITE OF CYTOCHROME P450 2B1: A STEERED MOLECULAR DYNAMICS SIMULATION. <i>Drug Metabolism and Disposition</i> , 2005, 33, 910-919.	1.7	50
33	Dynamic Allostery in the Methionine Repressor Revealed by Force Distribution Analysis. <i>PLoS Computational Biology</i> , 2009, 5, e1000574.	1.5	49
34	A novel calcium-binding site of von Willebrand factor A2 domain regulates its cleavage by ADAMTS13. <i>Blood</i> , 2011, 117, 4623-4631.	0.6	47
35	Structural basis of Focal Adhesion Kinase activation on lipid membranes. <i>EMBO Journal</i> , 2020, 39, e104743.	3.5	47
36	Mechano-redox control of integrin de-adhesion. <i>ELife</i> , 2018, 7, .	2.8	47

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37	Mutual A domain interactions in the force sensing protein von Willebrand factor. <i>Journal of Structural Biology</i> , 2017, 197, 57-64.	1.3	46
38	von Willebrand factor is dimerized by protein disulfide isomerase. <i>Blood</i> , 2016, 127, 1183-1191.	0.6	45
39	Evolutionary Optimization of Protein Folding. <i>PLoS Computational Biology</i> , 2013, 9, e1002861.	1.5	44
40	Origin of Orthogonality of Strain-Promoted Click Reactions. <i>Chemistry - A European Journal</i> , 2015, 21, 12431-12435.	1.7	44
41	Two Differential Binding Mechanisms of FG-Nucleoporins and Nuclear Transport Receptors. <i>Cell Reports</i> , 2018, 22, 3660-3671.	2.9	41
42	Identification of Allosteric Disulfides from Prestress Analysis. <i>Biophysical Journal</i> , 2014, 107, 672-681.	0.2	36
43	A fast recoiling silk-like elastomer facilitates nanosecond nematocyst discharge. <i>BMC Biology</i> , 2015, 13, 3.	1.7	34
44	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. <i>Journal of Membrane Biology</i> , 2018, 251, 609-631.	1.0	33
45	Allosteric Regulation of Focal Adhesion Kinase by PIP2 and ATP. <i>Biophysical Journal</i> , 2015, 108, 698-705.	0.2	32
46	How multisite phosphorylation impacts the conformations of intrinsically disordered proteins. <i>PLoS Computational Biology</i> , 2021, 17, e1008939.	1.5	32
47	Dissecting Entropic Coiling and Poor Solvent Effects in Protein Collapse. <i>Journal of the American Chemical Society</i> , 2008, 130, 11578-11579.	6.6	31
48	von Willebrand disease type 2A phenotypes IIC, IID and IIE: A day in the life of shear-stressed mutant von Willebrand factor. <i>Thrombosis and Haemostasis</i> , 2014, 112, 96-108.	1.8	31
49	Accessibility explains preferred thiol-disulfide isomerization in a protein domain. <i>Scientific Reports</i> , 2017, 7, 9858.	1.6	31
50	Dissecting the structural determinants for the difference in mechanical stability of silk and amyloid beta-sheet stacks. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 8765.	1.3	30
51	Ligand-Release Pathways in the Pheromone-Binding Protein of <i>Bombyx mori</i> . <i>Structure</i> , 2006, 14, 1567-1576.	1.6	29
52	Fluctuations of primary ubiquitin folding intermediates in a force clamp. <i>Journal of Structural Biology</i> , 2007, 157, 557-569.	1.3	28
53	Force Distribution Reveals Signal Transduction in <i>E. coli</i> Hsp90. <i>Biophysical Journal</i> , 2012, 103, 2195-2202.	0.2	28
54	Dynamic Prestress in a Globular Protein. <i>PLoS Computational Biology</i> , 2012, 8, e1002509.	1.5	28

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55	The mechano-sensing role of the unique SH3 insertion in plakin domains revealed by Molecular Dynamics simulations. <i>Scientific Reports</i> , 2017, 7, 11669.	1.6	28
56	Advances in molecular simulations of protein mechanical properties and function. <i>Current Opinion in Structural Biology</i> , 2020, 61, 132-138.	2.6	27
57	Rate-Dependent Behavior of the Amorphous Phase of Spider Dragline Silk. <i>Biophysical Journal</i> , 2014, 106, 2511-2518.	0.2	26
58	Mechanoradicals in tensed tendon collagen as a source of oxidative stress. <i>Nature Communications</i> , 2020, 11, 2315.	5.8	26
59	Exploring the Multidimensional Free Energy Surface of Phosphoester Hydrolysis with Constrained QM/MM Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3596-3604.	2.3	23
60	Protein mechanics: How force regulates molecular function. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013, 1830, 4762-4768.	1.1	23
61	Effects of crystalline subunit size on silk fiber mechanics. <i>Soft Matter</i> , 2011, 7, 8142.	1.2	22
62	Redox Potentials of Protein Disulfide Bonds from Free-Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5386-5391.	1.2	22
63	Sampling Long- versus Short-Range Interactions Defines the Ability of Force Fields To Reproduce the Dynamics of Intrinsically Disordered Proteins. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3964-3974.	2.3	22
64	On the mechanism of spontaneous thiolâ€“disulfide exchange in proteins. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16222-16230.	1.3	22
65	Structure and dynamics of the platelet integrin-binding C4 domain of von Willebrand factor. <i>Blood</i> , 2019, 133, 366-376.	0.6	22
66	Stress Propagation through Biological Lipid Bilayers in Silico. <i>Journal of the American Chemical Society</i> , 2017, 139, 13588-13591.	6.6	21
67	Isopeptide Bonds Mechanically Stabilize Spy0128 in Bacterial Pili. <i>Biophysical Journal</i> , 2013, 104, 2051-2057.	0.2	19
68	The plakin domain of <i>C. elegans</i> VAB-10/plectin acts as a hub in a mechanotransduction pathway to promote morphogenesis. <i>Development (Cambridge)</i> , 2019, 146, .	1.2	19
69	Glycosylation Enhances Peptide Hydrophobic Collapse by Impairing Solvation. <i>ChemPhysChem</i> , 2010, 11, 2367-2374.	1.0	18
70	Minicollagen cysteine-rich domains encode distinct modes of polymerization to form stable nematocyst capsules. <i>Scientific Reports</i> , 2016, 6, 25709.	1.6	18
71	Dynamic Allostery of the Catabolite Activator Protein Revealed by Interatomic Forces. <i>PLoS Computational Biology</i> , 2015, 11, e1004358.	1.5	18
72	Accurate Free Energies for Complex Condensed-Phase Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1213-1226.	2.3	18

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73	Controlling the Structure of Proteins at Surfaces. <i>Journal of the American Chemical Society</i> , 2010, 132, 17277-17281.	6.6	17
74	Base-Catalyzed Peptide Hydrolysis Is Insensitive to Mechanical Stress. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10126-10132.	1.2	17
75	An Allosteric Signaling Pathway of Human 3-Phosphoglycerate Kinase from Force Distribution Analysis. <i>PLoS Computational Biology</i> , 2014, 10, e1003444.	1.5	17
76	Graphene mechanics: II. Atomic stress distribution during indentation until rupture. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12582-12590.	1.3	17
77	Molecular Basis of the Mechanical Hierarchy in Myomesin Dimers for Sarcomere Integrity. <i>Biophysical Journal</i> , 2014, 107, 965-973.	0.2	17
78	How Fast Is Too Fast in Force-Probe Molecular Dynamics Simulations?. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3658-3664.	1.2	17
79	Minimum energy compact structures in force-quench polyubiquitin folding are domain swapped. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 6963-6968.	3.3	16
80	Viscous Friction between Crystalline and Amorphous Phase of Dragline Silk. <i>PLoS ONE</i> , 2014, 9, e104832.	1.1	16
81	Force distribution determines optimal length of $\beta^2$ -sheet crystals for mechanical robustness. <i>Soft Matter</i> , 2011, 7, 1308-1311.	1.2	15
82	Force Distribution Analysis of Mechanochemically Reactive Dimethylcyclobutene. <i>ChemPhysChem</i> , 2013, 14, 2687-2697.	1.0	15
83	Macromolecular Entropy Can Be Accurately Computed from Force. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4777-4781.	2.3	15
84	On the Cis to Trans Isomerization of Prolyl- $\epsilon$ -Peptide Bonds under Tension. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9346-9351.	1.2	14
85	How Fast Does a Signal Propagate through Proteins?. <i>PLoS ONE</i> , 2013, 8, e64746.	1.1	12
86	Mutation G1629E Increases von Willebrand Factor Cleavage via a Cooperative Destabilization Mechanism. <i>Biophysical Journal</i> , 2017, 112, 57-65.	0.2	11
87	Emergence of Hierarchical Modularity in Evolving Networks Uncovered by Phylogenomic Analysis. <i>Evolutionary Bioinformatics</i> , 2019, 15, 117693431987298.	0.6	11
88	Molecular Dynamics Simulations of Molecules in Uniform Flow. <i>Biophysical Journal</i> , 2019, 116, 1579-1585.	0.2	11
89	Graphene mechanics: I. Efficient first principles based Morse potential. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12591-12598.	1.3	10
90	Dynamic disorder can explain non-exponential kinetics of fast protein mechanical unfolding. <i>Journal of Structural Biology</i> , 2017, 197, 43-49.	1.3	10

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91	Entropy of flexible liquids from hierarchical force-torque covariance and coordination. <i>Molecular Physics</i> , 2018, 116, 1965-1976.	0.8	10
92	Hybrid Kinetic Monte Carlo/Molecular Dynamics Simulations of Bond Scissions in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 553-563.	2.3	10
93	ColBuilder: A server to build collagen fibril models. <i>Biophysical Journal</i> , 2021, 120, 3544-3549.	0.2	10
94	Probing molecular forces in multi-component physiological membranes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2155-2161.	1.3	10
95	Kinetic and structural roles for the surface in guiding SAS-6 self-assembly to direct centriole architecture. <i>Nature Communications</i> , 2021, 12, 6180.	5.8	10
96	Rupture Mechanism of Aromatic Systems from Graphite Probed with Molecular Dynamics Simulations. <i>Langmuir</i> , 2010, 26, 10791-10795.	1.6	8
97	Inositol hexakisphosphate increases the size of platelet aggregates. <i>Biochemical Pharmacology</i> , 2019, 161, 14-25.	2.0	8
98	Mechanical characterization and induced crystallization in nanocomposites of thermoplastics and carbon nanotubes. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	8
99	Bottom-up computational modeling of semi-crystalline fibers: from atomistic to continuum scale. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10426.	1.3	7
100	One-Way Allosteric Communication between the Two Disulfide Bonds in Tissue Factor. <i>Biophysical Journal</i> , 2017, 112, 78-86.	0.2	7
101	Stress-induced long-range ordering in spider silk. <i>Scientific Reports</i> , 2017, 7, 15273.	1.6	7
102	Phosphorylation tunes elongation propensity and cohesiveness of INCENP's intrinsically disordered region. <i>Journal of Molecular Biology</i> , 2022, 434, 167387.	2.0	7
103	Martini 3 coarse-grained force field for poly( <i>para</i> -phenylene ethynylene)s. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9998-10010.	1.3	7
104	A new method for the construction of coarse-grained models of large biomolecules from low-resolution cryo-electron microscopy data. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9720-9727.	1.3	6
105	Coarse-Grained Simulation of Mechanical Properties of Single Microtubules With Micrometer Length. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 632122.	1.6	6
106	Longitudinal strand ordering leads to shear thinning in Nafion. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25901-25910.	1.3	6
107	Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26366-26375.	1.3	6
108	Single molecule force spectroscopy data and BD- and MD simulations on the blood protein von Willebrand factor. <i>Data in Brief</i> , 2016, 8, 1080-1087.	0.5	5

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109	Organic Filling Mitigates Flaw-Sensitivity of Nanoscale Aragonite. ACS Biomaterials Science and Engineering, 2017, 3, 260-268.	2.6	5
110	Mechanical force can enhance c-Src kinase activity by impairing autoinhibition. Biophysical Journal, 2022, 121, 684-691.	0.2	5
111	ATP allosterically stabilizes integrin-linked kinase for efficient force generation. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2106098119.	3.3	5
112	Force Propagation in Proteins From Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 589a.	0.2	3
113	Stability of Biological Membranes upon Mechanical Indentation. Journal of Physical Chemistry B, 2018, 122, 7073-7079.	1.2	3
114	Studying Functional Disulphide Bonds by Computer Simulations. Methods in Molecular Biology, 2019, 1967, 87-113.	0.4	3
115	How ARVC-Related Mutations Destabilize Desmoplakin: An MD Study. Biophysical Journal, 2019, 116, 831-835.	0.2	3
116	Gain-of-Function Variant p.Pro2555Arg of von Willebrand Factor Increases Aggregate Size through Altering Stem Dynamics. Thrombosis and Haemostasis, 2020, , .	1.8	3
117	Transition Path Sampling with Quantum/Classical Mechanics for Reaction Rates. Methods in Molecular Biology, 2015, 1215, 27-45.	0.4	2
118	Mechanosensation through Radicals in Tensed Collagen. Biophysical Journal, 2018, 114, 113a.	0.2	1
119	How Collagen Fibrils Dynamically Distribute and Measure Stresses. Biophysical Journal, 2018, 114, 398a-399a.	0.2	1
120	Force Distribution in Proteins from Molecular Dynamics Simulations. , 2009, , .		0
121	Single-Molecule Force Spectroscopy Reveals the Function of Titin Kinase as Force Sensor. Biophysical Journal, 2009, 96, 643a.	0.2	0
122	Multi-Scale Modeling of Force Propagation in Proteins Under Mechanical Stress. Biophysical Journal, 2010, 98, 596a.	0.2	0
123	Nano-Scale Mechanics of Nacre: Forces at Protein-Crystal Linkages and Flaws. Biophysical Journal, 2012, 102, 733a-734a.	0.2	0
124	Force-Dependent Platelet Binding of the Von Willebrand Factor A1-A2 Complex from Atomistic Simulations. Biophysical Journal, 2013, 104, 58a.	0.2	0
125	Prestress in Protein Disulfide Bonds Tunes their Stabilities. Biophysical Journal, 2013, 104, 58a-59a.	0.2	0
126	An Allosteric Signaling Pathway of Human 3-Phosphoglycerate Kinase. Biophysical Journal, 2014, 106, 610a.	0.2	0

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127	Mechanosignalling of Focal Adhesion Kinase. Biophysical Journal, 2015, 108, 506a.	0.2	0
128	Simulating Force Response at Cellular Junctions: Desmoplakin as a Molecular Force Sensor?. Biophysical Journal, 2017, 112, 195a-196a.	0.2	0
129	Mechano-Induced Unfolding of Von Willebrand Factor: A Clinical Example of Protein Destabilization. Biophysical Journal, 2017, 112, 490a.	0.2	0
130	Towards Simulating Large-Scale Self-Assembly of Proteins under Flow. Biophysical Journal, 2017, 112, 592a-593a.	0.2	0
131	Stress Propagation through Biological Lipid-Bilayers Revealed by Atomistic and Coarse-Grained Simulations. Biophysical Journal, 2017, 112, 76a.	0.2	0
132	Punching Membranes: How Lipid Bilayers Withstand and Propagate Mechanical Load. Biophysical Journal, 2018, 114, 562a.	0.2	0
133	When an Enzyme Self-Assembles on a Membrane: Focal Adhesion Kinase. Biophysical Journal, 2018, 114, 61a.	0.2	0