Frauke Grter

List of Publications by Year in Descending Order

115 papers	5,680 citations	35 h-index	73 g-index
138 ext. papers	6,625 ext. citations	5.8 avg, IF	5.5 L-index

#	Paper	IF	Citations
115	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	11.5	1
114	Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. *Physical Chemistry Chemical Physics*, **2021**, 23, 26366-26375	3.6	0
113	Longitudinal strand ordering leads to shear thinning in Nafion. *Physical Chemistry Chemical Physics*, **2021**, 23, 25901-25910	3.6	0
112	Phosphorylation tunes elongation propensity and cohesiveness of INCENP's intrinsically disordered region. *Journal of Molecular Biology*, **2021**, 434, 167387	6.5	0
111	Kinetic and structural roles for the surface in guiding SAS-6 self-assembly to direct centriole architecture. *Nature Communications*, **2021**, 12, 6180	17.4	3
110	How multisite phosphorylation impacts the conformations of intrinsically disordered proteins. *PLoS Computational Biology*, **2021**, 17, e1008939	5	7
109	ColBuilder: A server to build collagen fibril models. *Biophysical Journal*, **2021**, 120, 3544-3549	2.9	0
108	Mechanoradicals in tensed tendon collagen as a source of oxidative stress. *Nature Communications*, **2020**, 11, 2315	17.4	10
107	Advances in molecular simulations of protein mechanical properties and function. *Current Opinion in Structural Biology*, **2020**, 61, 132-138	8.1	11
106	Structural basis of Focal Adhesion Kinase activation on lipid membranes. *EMBO Journal*, **2020**, 39, e104743	13	17
105	Hybrid Kinetic Monte Carlo/Molecular Dynamics Simulations of Bond Scissions in Proteins. *Journal of Chemical Theory and Computation*, **2020**, 16, 553-563	6.4	5
104	Mechanical characterization and induced crystallization in nanocomposites of thermoplastics and carbon nanotubes. *Npj Computational Materials*, **2020**, 6,	10.9	3
103	Coarse-Grained Simulation of Mechanical Properties of Single Microtubules With Micrometer Length. *Frontiers in Molecular Biosciences*, **2020**, 7, 632122	5.6	1
102	Studying Functional Disulphide Bonds by Computer Simulations. *Methods in Molecular Biology*, **2019**, 1967, 87-113	1.4	3
101	Molecular Dynamics Simulations of Molecules in Uniform Flow. *Biophysical Journal*, **2019**, 116, 1579-1585	2.9	6
100	A new method for the construction of coarse-grained models of large biomolecules from low-resolution cryo-electron microscopy data. *Physical Chemistry Chemical Physics*, **2019**, 21, 9720-9727	3.6	3
99	Structural and mechanistic insights into mechanoactivation of focal adhesion kinase. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 6766-6774	11.5	48

98	How Fast Is Too Fast in Force-Probe Molecular Dynamics Simulations?. *Journal of Physical Chemistry B*, **2019**, 123, 3658-3664	3.4	10
97	How ARVC-Related Mutations Destabilize Desmoplakin: An MD Study. *Biophysical Journal*, **2019**, 116, 831-835	2.9	2
96	Emergence of Hierarchical Modularity in Evolving Networks Uncovered by Phylogenomic Analysis. *Evolutionary Bioinformatics*, **2019**, 15, 1176934319872980	1.9	5
95	The plakin domain of VAB-10/plectin acts as a hub in a mechanotransduction pathway to promote morphogenesis. *Development (Cambridge)*, **2019**, 146,	6.6	13
94	Inositol hexakisphosphate increases the size of platelet aggregates. *Biochemical Pharmacology*, **2019**, 161, 14-25	6	5
93	Structure and dynamics of the platelet integrin-binding C4 domain of von Willebrand factor. *Blood*, **2019**, 133, 366-376	2.2	9
92	Autoregulation of von Willebrand factor function by a disulfide bond switch. *Science Advances*, **2018**, 4, eaaq1477	14.3	56
91	CONAN: A Tool to Decode Dynamical Information from Molecular Interaction Maps. *Biophysical Journal*, **2018**, 114, 1267-1273	2.9	36
90	Two Differential Binding Mechanisms of FG-Nucleoporins and Nuclear Transport Receptors. *Cell Reports*, **2018**, 22, 3660-3671	10.6	28
89	Protein S-Bacillithiolation Functions in Thiol Protection and Redox Regulation of the Glyceraldehyde-3-Phosphate Dehydrogenase Gap in Staphylococcus aureus Under Hypochlorite Stress. *Antioxidants and Redox Signaling*, **2018**, 28, 410-430	8.4	39
88	Stability of Biological Membranes upon Mechanical Indentation. *Journal of Physical Chemistry B*, **2018**, 122, 7073-7079	3.4	3
87	Mechano-redox control of integrin de-adhesion. *ELife*, **2018**, 7,	8.9	33
86	Probing molecular forces in multi-component physiological membranes. *Physical Chemistry Chemical Physics*, **2018**, 20, 2155-2161	3.6	7
85	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. *Journal of Membrane Biology*, **2018**, 251, 609-631	2.3	26
84	On the mechanism of spontaneous thiol-disulfide exchange in proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 16222-16230	3.6	12
83	Entropy of flexible liquids from hierarchical force□torque covariance and coordination. *Molecular Physics*, **2018**, 116, 1965-1976	1.7	7
82	Mutual A domain interactions in the force sensing protein von Willebrand factor. *Journal of Structural Biology*, **2017**, 197, 57-64	3.4	19
81	Dynamic disorder can explain non-exponential kinetics of fast protein mechanical unfolding. *Journal of Structural Biology*, **2017**, 197, 43-49	3.4	9

80	Mutation G1629E Increases von Willebrand Factor Cleavage via a Cooperative Destabilization Mechanism. *Biophysical Journal*, **2017**, 112, 57-65	2.9	7
79	One-Way Allosteric Communication between the Two Disulfide Bonds in Tissue Factor. *Biophysical Journal*, **2017**, 112, 78-86	2.9	7
78	Organic Filling Mitigates Flaw-Sensitivity of Nanoscale Aragonite. *ACS Biomaterials Science and Engineering*, **2017**, 3, 260-268	5.5	5
77	Stress Propagation through Biological Lipid Bilayers in Silico. *Journal of the American Chemical Society*, **2017**, 139, 13588-13591	16.4	20
76	The mechano-sensing role of the unique SH3 insertion in plakin domains revealed by Molecular Dynamics simulations. *Scientific Reports*, **2017**, 7, 11669	4.9	19
75	Accessibility explains preferred thiol-disulfide isomerization in a protein domain. *Scientific Reports*, **2017**, 7, 9858	4.9	16
74	Decoupling of size and shape fluctuations in heteropolymeric sequences reconciles discrepancies in SAXS vs. FRET measurements. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E6342-E6351	11.5	136
73	Sampling Long- versus Short-Range Interactions Defines the Ability of Force Fields To Reproduce the Dynamics of Intrinsically Disordered Proteins. *Journal of Chemical Theory and Computation*, **2017**, 13, 3964-3974	6.4	15
72	Stress-induced long-range ordering in spider silk. *Scientific Reports*, **2017**, 7, 15273	4.9	4
71	Minicollagen cysteine-rich domains encode distinct modes of polymerization to form stable nematocyst capsules. *Scientific Reports*, **2016**, 6, 25709	4.9	11
70	von Willebrand factor is dimerized by protein disulfide isomerase. *Blood*, **2016**, 127, 1183-91	2.2	33
69	Single molecule force spectroscopy data and BD- and MD simulations on the blood protein von Willebrand factor. *Data in Brief*, **2016**, 8, 1080-7	1.2	3
68	A fast recoiling silk-like elastomer facilitates nanosecond nematocyst discharge. *BMC Biology*, **2015**, 13, 3	7.3	26
67	Redox potentials of protein disulfide bonds from free-energy calculations. *Journal of Physical Chemistry B*, **2015**, 119, 5386-91	3.4	16
66	Origin of Orthogonality of Strain-Promoted Click Reactions. *Chemistry - A European Journal*, **2015**, 21, 12431-5	4.8	40
65	Force-sensitive autoinhibition of the von Willebrand factor is mediated by interdomain interactions. *Biophysical Journal*, **2015**, 108, 2312-21	2.9	49
64	Kirkwood-Buff Approach Rescues Overcollapse of a Disordered Protein in Canonical Protein Force Fields. *Journal of Physical Chemistry B*, **2015**, 119, 7975-84	3.4	61
63	Plasticity of an ultrafast interaction between nucleoporins and nuclear transport receptors. *Cell*, **2015**, 163, 734-45	56.2	185

62	Allosteric regulation of focal adhesion kinase by PIP and ATP. *Biophysical Journal*, **2015**, 108, 698-705	2.9	29
61	A proton relay enhances H2O2 sensitivity of GAPDH to facilitate metabolic adaptation. *Nature Chemical Biology*, **2015**, 11, 156-63	11.7	136
60	Dynamic Allostery of the Catabolite Activator Protein Revealed by Interatomic Forces. *PLoS Computational Biology*, **2015**, 11, e1004358	5	13
59	Mechanism of Focal Adhesion Kinase Mechanosensing. *PLoS Computational Biology*, **2015**, 11, e1004593	5	70
58	Transition path sampling with quantum/classical mechanics for reaction rates. *Methods in Molecular Biology*, **2015**, 1215, 27-45	1.4	2
57	von Willebrand factor directly interacts with DNA from neutrophil extracellular traps. *Arteriosclerosis, Thrombosis, and Vascular Biology*, **2014**, 34, 1382-9	9.4	97
56	Macromolecular Entropy Can Be Accurately Computed from Force. *Journal of Chemical Theory and Computation*, **2014**, 10, 4777-81	6.4	11
55	Graphene mechanics: II. Atomic stress distribution during indentation until rupture. *Physical Chemistry Chemical Physics*, **2014**, 16, 12582-90	3.6	17
54	Molecular basis of the mechanical hierarchy in myomesin dimers for sarcomere integrity. *Biophysical Journal*, **2014**, 107, 965-73	2.9	15
53	Identification of allosteric disulfides from prestress analysis. *Biophysical Journal*, **2014**, 107, 672-681	2.9	32
52	Graphene mechanics: I. Efficient first principles based Morse potential. *Physical Chemistry Chemical Physics*, **2014**, 16, 12591-8	3.6	7
51	Rate-dependent behavior of the amorphous phase of spider dragline silk. *Biophysical Journal*, **2014**, 106, 2511-8	2.9	23
50	von Willebrand disease type 2A phenotypes IIC, IID and IIE: A day in the life of shear-stressed mutant von Willebrand factor. *Thrombosis and Haemostasis*, **2014**, 112, 96-108	7	23
49	Phosphatidylinositol 4,5-bisphosphate triggers activation of focal adhesion kinase by inducing clustering and conformational changes. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E3177-86	11.5	81
48	An allosteric signaling pathway of human 3-phosphoglycerate kinase from force distribution analysis. *PLoS Computational Biology*, **2014**, 10, e1003444	5	16
47	Viscous friction between crystalline and amorphous phase of dragline silk. *PLoS ONE*, **2014**, 9, e104832	3.7	13
46	Force distribution analysis of mechanochemically reactive dimethylcyclobutene. *ChemPhysChem*, **2013**, 14, 2687-97	3.2	14
45	Time-resolved force distribution analysis. *BMC Biophysics*, **2013**, 6, 5	0	39

44	Isopeptide bonds mechanically stabilize spy0128 in bacterial pili. *Biophysical Journal*, **2013**, 104, 2051-7	2.9	16
43	Protein mechanics: how force regulates molecular function. *Biochimica Et Biophysica Acta - General Subjects*, **2013**, 1830, 4762-8	4	21
42	Evolutionary optimization of protein folding. *PLoS Computational Biology*, **2013**, 9, e1002861	5	35
41	Dissecting the structural determinants for the difference in mechanical stability of silk and amyloid beta-sheet stacks. *Physical Chemistry Chemical Physics*, **2013**, 15, 8765-71	3.6	20
40	How fast does a signal propagate through proteins?. *PLoS ONE*, **2013**, 8, e64746	3.7	12
39	On the cis to trans isomerization of prolyl-peptide bonds under tension. *Journal of Physical Chemistry B*, **2012**, 116, 9346-51	3.4	14
38	Exploring the Multidimensional Free Energy Surface of Phosphoester Hydrolysis with Constrained QM/MM Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 3596-604	6.4	22
37	Mechanical force can fine-tune redox potentials of disulfide bonds. *Biophysical Journal*, **2012**, 102, 622-9	2.9	42
36	Force distribution reveals signal transduction in E. coli Hsp90. *Biophysical Journal*, **2012**, 103, 2195-202	2.9	23
35	Dynamic prestress in a globular protein. *PLoS Computational Biology*, **2012**, 8, e1002509	5	23
34	Silk fiber mechanics from multiscale force distribution analysis. *Biophysical Journal*, **2011**, 100, 1298-305	2.9	59
33	Strained Molecules: Insights from Force Distribution Analysis **2011**, 301-310		
32	Effects of crystalline subunit size on silk fiber mechanics. *Soft Matter*, **2011**, 7, 8142	3.6	19
31	A New Transferable Forcefield for Simulating the Mechanics of CaCO3Crystals. *Journal of Physical Chemistry C*, **2011**, 115, 20067-20075	3.8	75
30	A novel calcium-binding site of von Willebrand factor A2 domain regulates its cleavage by ADAMTS13. *Blood*, **2011**, 117, 4623-31	2.2	41
29	Force distribution determines optimal length of β-sheet crystals for mechanical robustness. *Soft Matter*, **2011**, 7, 1308-1311	3.6	13
28	Bottom-up computational modeling of semi-crystalline fibers: from atomistic to continuum scale. *Physical Chemistry Chemical Physics*, **2011**, 13, 10426-9	3.6	7
27	Base-catalyzed peptide hydrolysis is insensitive to mechanical stress. *Journal of Physical Chemistry B* , **2011**, 115, 10126-32	3.4	17

26	Fast-folding alpha-helices as reversible strain absorbers in the muscle protein myomesin. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 14139-44	11.5	50
25	Minimum energy compact structures in force-quench polyubiquitin folding are domain swapped. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6963-8	11.5	14
24	Unique amino acid signatures that are evolutionarily conserved distinguish simple-type, epidermal and hair keratins. *Journal of Cell Science*, **2011**, 124, 4221-32	5.3	51
23	How sequence determines elasticity of disordered proteins. *Biophysical Journal*, **2010**, 99, 3863-9	2.9	50
22	Rupture mechanism of aromatic systems from graphite probed with molecular dynamics simulations. *Langmuir*, **2010**, 26, 10791-5	4	6
21	Controlling the structure of proteins at surfaces. *Journal of the American Chemical Society*, **2010**, 132, 17277-81	16.4	14
20	Atomistic evidence of how force dynamically regulates thiol/disulfide exchange. *Journal of the American Chemical Society*, **2010**, 132, 16790-5	16.4	55
19	Glycosylation enhances peptide hydrophobic collapse by impairing solvation. *ChemPhysChem*, **2010**, 11, 2367-74	3.2	16
18	Mechanical network in titin immunoglobulin from force distribution analysis. *PLoS Computational Biology*, **2009**, 5, e1000306	5	58
17	Dynamic allostery in the methionine repressor revealed by force distribution analysis. *PLoS Computational Biology*, **2009**, 5, e1000574	5	48
16	Shear-induced unfolding activates von Willebrand factor A2 domain for proteolysis. *Journal of Thrombosis and Haemostasis*, **2009**, 7, 2096-105	15.4	94
15	Mechanical response of silk crystalline units from force-distribution analysis. *Biophysical Journal*, **2009**, 96, 3997-4005	2.9	86
14	Force Propagation in Proteins From Molecular Dynamics Simulations. *Biophysical Journal*, **2009**, 96, 589a	2.9	2
13	Dissecting entropic coiling and poor solvent effects in protein collapse. *Journal of the American Chemical Society*, **2008**, 130, 11578-9	16.4	28
12	Mechanoenzymatics of titin kinase. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 13385-90	11.5	280
11	Signatures of hydrophobic collapse in extended proteins captured with force spectroscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 7916-21	11.5	87
10	Probing the chemistry of thioredoxin catalysis with force. *Nature*, **2007**, 450, 124-7	50.4	224
9	Fluctuations of primary ubiquitin folding intermediates in a force clamp. *Journal of Structural Biology*, **2007**, 157, 557-69	3.4	27

8	Ligand-release pathways in the pheromone-binding protein of Bombyx mori. *Structure*, **2006**, 14, 1567-76	5.2	29
7	Pheromone discrimination by the pheromone-binding protein of Bombyx mori. *Structure*, **2006**, 14, 1577-86	5.2	52
6	Molecular anatomy of a trafficking organelle. *Cell*, **2006**, 127, 831-46	56.2	1670
5	Mechanically induced titin kinase activation studied by force-probe molecular dynamics simulations. *Biophysical Journal*, **2005**, 88, 790-804	2.9	181
4	Protein/ligand binding free energies calculated with quantum mechanics/molecular mechanics. *Journal of Physical Chemistry B*, **2005**, 109, 10474-83	3.4	92
3	Structure and mechanism of the reversible photoswitch of a fluorescent protein. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 13070-4	11.5	222
2	Possible pathway(s) of testosterone egress from the active site of cytochrome P450 2B1: a steered molecular dynamics simulation. *Drug Metabolism and Disposition*, **2005**, 33, 910-9	4	45
1	Surface-catalyzed SAS-6 self-assembly directs centriole formation through kinetic and structural mechanisms		5