

Frauke Grter

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Molecular anatomy of a trafficking organelle. <i>Cell</i> , 2006 , 127, 831-46	56.2	1670
114	Mechanoenzymatics of titin kinase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 13385-90	11.5	280
113	Probing the chemistry of thioredoxin catalysis with force. <i>Nature</i> , 2007 , 450, 124-7	50.4	224
112	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, 13070-4	11.5	222
111	Plasticity of an ultrafast interaction between nucleoporins and nuclear transport receptors. <i>Cell</i> , 2015 , 163, 734-45	56.2	185
110	Mechanically induced titin kinase activation studied by force-probe molecular dynamics simulations. <i>Biophysical Journal</i> , 2005 , 88, 790-804	2.9	181
109	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	11.5	136
108	A proton relay enhances H ₂ O ₂ sensitivity of GAPDH to facilitate metabolic adaptation. <i>Nature Chemical Biology</i> , 2015 , 11, 156-63	11.7	136
107	von Willebrand factor directly interacts with DNA from neutrophil extracellular traps. <i>Arteriosclerosis, Thrombosis, and Vascular Biology</i> , 2014 , 34, 1382-9	9.4	97
106	Shear-induced unfolding activates von Willebrand factor A2 domain for proteolysis. <i>Journal of Thrombosis and Haemostasis</i> , 2009 , 7, 2096-105	15.4	94
105	Protein/ligand binding free energies calculated with quantum mechanics/molecular mechanics. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 10474-83	3.4	92
104	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, 7916-21	11.5	87
103	Mechanical response of silk crystalline units from force-distribution analysis. <i>Biophysical Journal</i> , 2009 , 96, 3997-4005	2.9	86
102	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	11.5	81
101	A New Transferable Forcefield for Simulating the Mechanics of CaCO ₃ Crystals. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 20067-20075	3.8	75
100	Mechanism of Focal Adhesion Kinase Mechanosensing. <i>PLoS Computational Biology</i> , 2015 , 11, e1004593	5	70
99	Kirkwood-Buff Approach Rescues Overcollapse of a Disordered Protein in Canonical Protein Force Fields. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 7975-84	3.4	61

98	Silk fiber mechanics from multiscale force distribution analysis. <i>Biophysical Journal</i> , 2011 , 100, 1298-305	2.9	59
97	Mechanical network in titin immunoglobulin from force distribution analysis. <i>PLoS Computational Biology</i> , 2009 , 5, e1000306	5	58
96	Autoregulation of von Willebrand factor function by a disulfide bond switch. <i>Science Advances</i> , 2018 , 4, eaaq1477	14.3	56
95	Atomistic evidence of how force dynamically regulates thiol/disulfide exchange. <i>Journal of the American Chemical Society</i> , 2010 , 132, 16790-5	16.4	55
94	Pheromone discrimination by the pheromone-binding protein of <i>Bombyx mori</i> . <i>Structure</i> , 2006 , 14, 1577-86	5.86	52
93	Unique amino acid signatures that are evolutionarily conserved distinguish simple-type, epidermal and hair keratins. <i>Journal of Cell Science</i> , 2011 , 124, 4221-32	5.3	51
92	How sequence determines elasticity of disordered proteins. <i>Biophysical Journal</i> , 2010 , 99, 3863-9	2.9	50
91	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, 14139-44	11.5	50
90	Force-sensitive autoinhibition of the von Willebrand factor is mediated by interdomain interactions. <i>Biophysical Journal</i> , 2015 , 108, 2312-21	2.9	49
89	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	11.5	48
88	Dynamic allostery in the methionine repressor revealed by force distribution analysis. <i>PLoS Computational Biology</i> , 2009 , 5, e1000574	5	48
87	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, 910-9	4	45
86	Mechanical force can fine-tune redox potentials of disulfide bonds. <i>Biophysical Journal</i> , 2012 , 102, 622-9	2.9	42
85	A novel calcium-binding site of von Willebrand factor A2 domain regulates its cleavage by ADAMTS13. <i>Blood</i> , 2011 , 117, 4623-31	2.2	41
84	Origin of Orthogonality of Strain-Promoted Click Reactions. <i>Chemistry - A European Journal</i> , 2015 , 21, 12431-5	4.8	40
83	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	8.4	39
82	Time-resolved force distribution analysis. <i>BMC Biophysics</i> , 2013 , 6, 5	0	39
81	CONAN: A Tool to Decode Dynamical Information from Molecular Interaction Maps. <i>Biophysical Journal</i> , 2018 , 114, 1267-1273	2.9	36

80	Evolutionary optimization of protein folding. <i>PLoS Computational Biology</i> , 2013 , 9, e1002861	5	35
79	von Willebrand factor is dimerized by protein disulfide isomerase. <i>Blood</i> , 2016 , 127, 1183-91	2.2	33
78	Mechano-redox control of integrin de-adhesion. <i>ELife</i> , 2018 , 7,	8.9	33
77	Identification of allosteric disulfides from prestress analysis. <i>Biophysical Journal</i> , 2014 , 107, 672-681	2.9	32
76	Allosteric regulation of focal adhesion kinase by PI3K and ATP. <i>Biophysical Journal</i> , 2015 , 108, 698-705	2.9	29
75	Ligand-release pathways in the pheromone-binding protein of <i>Bombyx mori</i> . <i>Structure</i> , 2006 , 14, 1567-76	6.2	29
74	Two Differential Binding Mechanisms of FG-Nucleoporins and Nuclear Transport Receptors. <i>Cell Reports</i> , 2018 , 22, 3660-3671	10.6	28
73	Dissecting entropic coiling and poor solvent effects in protein collapse. <i>Journal of the American Chemical Society</i> , 2008 , 130, 11578-9	16.4	28
72	Fluctuations of primary ubiquitin folding intermediates in a force clamp. <i>Journal of Structural Biology</i> , 2007 , 157, 557-69	3.4	27
71	A fast recoiling silk-like elastomer facilitates nanosecond nematocyst discharge. <i>BMC Biology</i> , 2015 , 13, 3	7.3	26
70	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. <i>Journal of Membrane Biology</i> , 2018 , 251, 609-631	2.3	26
69	Rate-dependent behavior of the amorphous phase of spider dragline silk. <i>Biophysical Journal</i> , 2014 , 106, 2511-8	2.9	23
68	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	7	23
67	Force distribution reveals signal transduction in <i>E. coli</i> Hsp90. <i>Biophysical Journal</i> , 2012 , 103, 2195-202	2.9	23
66	Dynamic prestress in a globular protein. <i>PLoS Computational Biology</i> , 2012 , 8, e1002509	5	23
65	Exploring the Multidimensional Free Energy Surface of Phosphoester Hydrolysis with Constrained QM/MM Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3596-604	6.4	22
64	Protein mechanics: how force regulates molecular function. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013 , 1830, 4762-8	4	21
63	Stress Propagation through Biological Lipid Bilayers in Silico. <i>Journal of the American Chemical Society</i> , 2017 , 139, 13588-13591	16.4	20

62	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, 8765-71	3.6	20
61	Mutual A domain interactions in the force sensing protein von Willebrand factor. <i>Journal of Structural Biology</i> , 2017 , 197, 57-64	3.4	19
60	The mechano-sensing role of the unique SH3 insertion in plakin domains revealed by Molecular Dynamics simulations. <i>Scientific Reports</i> , 2017 , 7, 11669	4.9	19
59	Effects of crystalline subunit size on silk fiber mechanics. <i>Soft Matter</i> , 2011 , 7, 8142	3.6	19
58	Graphene mechanics: II. Atomic stress distribution during indentation until rupture. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 12582-90	3.6	17
57	Base-catalyzed peptide hydrolysis is insensitive to mechanical stress. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 10126-32	3.4	17
56	Structural basis of Focal Adhesion Kinase activation on lipid membranes. <i>EMBO Journal</i> , 2020 , 39, e104743	4.3	17
55	Redox potentials of protein disulfide bonds from free-energy calculations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 5386-91	3.4	16
54	Isopeptide bonds mechanically stabilize spy0128 in bacterial pili. <i>Biophysical Journal</i> , 2013 , 104, 2051-7	2.9	16
53	Accessibility explains preferred thiol-disulfide isomerization in a protein domain. <i>Scientific Reports</i> , 2017 , 7, 9858	4.9	16
52	An allosteric signaling pathway of human 3-phosphoglycerate kinase from force distribution analysis. <i>PLoS Computational Biology</i> , 2014 , 10, e1003444	5	16
51	Glycosylation enhances peptide hydrophobic collapse by impairing solvation. <i>ChemPhysChem</i> , 2010 , 11, 2367-74	3.2	16
50	Molecular basis of the mechanical hierarchy in myomesin dimers for sarcomere integrity. <i>Biophysical Journal</i> , 2014 , 107, 965-73	2.9	15
49	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	6.4	15
48	Force distribution analysis of mechanochemically reactive dimethylcyclobutene. <i>ChemPhysChem</i> , 2013 , 14, 2687-97	3.2	14
47	On the cis to trans isomerization of prolyl-peptide bonds under tension. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 9346-51	3.4	14
46	Controlling the structure of proteins at surfaces. <i>Journal of the American Chemical Society</i> , 2010 , 132, 17277-81	16.4	14
45	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, 6963-8	11.5	14

44	Force distribution determines optimal length of Esheet crystals for mechanical robustness. <i>Soft Matter</i> , 2011 , 7, 1308-1311	3.6	13
43	Dynamic Allostery of the Catabolite Activator Protein Revealed by Interatomic Forces. <i>PLoS Computational Biology</i> , 2015 , 11, e1004358	5	13
42	Viscous friction between crystalline and amorphous phase of dragline silk. <i>PLoS ONE</i> , 2014 , 9, e104832	3.7	13
41	The plakin domain of VAB-10/plectin acts as a hub in a mechanotransduction pathway to promote morphogenesis. <i>Development (Cambridge)</i> , 2019 , 146,	6.6	13
40	How fast does a signal propagate through proteins?. <i>PLoS ONE</i> , 2013 , 8, e64746	3.7	12
39	On the mechanism of spontaneous thiol-disulfide exchange in proteins. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 16222-16230	3.6	12
38	Advances in molecular simulations of protein mechanical properties and function. <i>Current Opinion in Structural Biology</i> , 2020 , 61, 132-138	8.1	11
37	Minicollagen cysteine-rich domains encode distinct modes of polymerization to form stable nematocyst capsules. <i>Scientific Reports</i> , 2016 , 6, 25709	4.9	11
36	Macromolecular Entropy Can Be Accurately Computed from Force. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4777-81	6.4	11
35	How Fast Is Too Fast in Force-Probe Molecular Dynamics Simulations?. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 3658-3664	3.4	10
34	Mechanoradicals in tensed tendon collagen as a source of oxidative stress. <i>Nature Communications</i> , 2020 , 11, 2315	17.4	10
33	Dynamic disorder can explain non-exponential kinetics of fast protein mechanical unfolding. <i>Journal of Structural Biology</i> , 2017 , 197, 43-49	3.4	9
32	Structure and dynamics of the platelet integrin-binding C4 domain of von Willebrand factor. <i>Blood</i> , 2019 , 133, 366-376	2.2	9
31	Mutation G1629E Increases von Willebrand Factor Cleavage via a Cooperative Destabilization Mechanism. <i>Biophysical Journal</i> , 2017 , 112, 57-65	2.9	7
30	One-Way Allosteric Communication between the Two Disulfide Bonds in Tissue Factor. <i>Biophysical Journal</i> , 2017 , 112, 78-86	2.9	7
29	Graphene mechanics: I. Efficient first principles based Morse potential. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 12591-8	3.6	7
28	Bottom-up computational modeling of semi-crystalline fibers: from atomistic to continuum scale. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 10426-9	3.6	7
27	Probing molecular forces in multi-component physiological membranes. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 2155-2161	3.6	7

26	How multisite phosphorylation impacts the conformations of intrinsically disordered proteins. <i>PLoS Computational Biology</i> , 2021 , 17, e1008939	5	7
25	Entropy of flexible liquids from hierarchical force-torque covariance and coordination. <i>Molecular Physics</i> , 2018 , 116, 1965-1976	1.7	7
24	Molecular Dynamics Simulations of Molecules in Uniform Flow. <i>Biophysical Journal</i> , 2019 , 116, 1579-1585.	5.9	6
23	Rupture mechanism of aromatic systems from graphite probed with molecular dynamics simulations. <i>Langmuir</i> , 2010 , 26, 10791-5	4	6
22	Organic Filling Mitigates Flaw-Sensitivity of Nanoscale Aragonite. <i>ACS Biomaterials Science and Engineering</i> , 2017 , 3, 260-268	5.5	5
21	Emergence of Hierarchical Modularity in Evolving Networks Uncovered by Phylogenomic Analysis. <i>Evolutionary Bioinformatics</i> , 2019 , 15, 1176934319872980	1.9	5
20	Surface-catalyzed SAS-6 self-assembly directs centriole formation through kinetic and structural mechanisms	5	
19	Hybrid Kinetic Monte Carlo/Molecular Dynamics Simulations of Bond Scissions in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 553-563	6.4	5
18	Inositol hexakisphosphate increases the size of platelet aggregates. <i>Biochemical Pharmacology</i> , 2019 , 161, 14-25	6	5
17	Stress-induced long-range ordering in spider silk. <i>Scientific Reports</i> , 2017 , 7, 15273	4.9	4
16	Studying Functional Disulphide Bonds by Computer Simulations. <i>Methods in Molecular Biology</i> , 2019 , 1967, 87-113	1.4	3
15	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	3.6	3
14	Stability of Biological Membranes upon Mechanical Indentation. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7073-7079	3.4	3
13	Kinetic and structural roles for the surface in guiding SAS-6 self-assembly to direct centriole architecture. <i>Nature Communications</i> , 2021 , 12, 6180	17.4	3
12	Mechanical characterization and induced crystallization in nanocomposites of thermoplastics and carbon nanotubes. <i>Npj Computational Materials</i> , 2020 , 6,	10.9	3
11	Single molecule force spectroscopy data and BD- and MD simulations on the blood protein von Willebrand factor. <i>Data in Brief</i> , 2016 , 8, 1080-7	1.2	3
10	How ARVC-Related Mutations Destabilize Desmoplakin: An MD Study. <i>Biophysical Journal</i> , 2019 , 116, 831-835	2.9	2
9	Force Propagation in Proteins From Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2009 , 96, 589a2.9	2.9	2

8	Transition path sampling with quantum/classical mechanics for reaction rates. <i>Methods in Molecular Biology</i> , 2015 , 1215, 27-45	1.4	2
7	Coarse-Grained Simulation of Mechanical Properties of Single Microtubules With Micrometer Length. <i>Frontiers in Molecular Biosciences</i> , 2020 , 7, 632122	5.6	1
6	ATP allosterically stabilizes integrin-linked kinase for efficient force generation.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022 , 119, e2106098119	11.5	1
5	Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 26366-26375	3.6	0
4	Longitudinal strand ordering leads to shear thinning in Nafion. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 25901-25910	3.6	0
3	Phosphorylation tunes elongation propensity and cohesiveness of INCENP's intrinsically disordered region. <i>Journal of Molecular Biology</i> , 2021 , 434, 167387	6.5	0
2	ColBuilder: A server to build collagen fibril models. <i>Biophysical Journal</i> , 2021 , 120, 3544-3549	2.9	0
1	Strained Molecules: Insights from Force Distribution Analysis 2011 , 301-310		