Garegin A Papoian

List of Publications by Year
in descending order

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96 papers	4,560 citations	117453 34 h-index	114278 63 g-index
120 all docs	120 docs citations	120 times ranked	4196 citing authors

#	Article	IF	Citations
1	From The Cover: Water in protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 3352-3357.	3.3	293
2	AWSEM-MD: Protein Structure Prediction Using Coarse-Grained Physical Potentials and Bioinformatically Based Local Structure Biasing. Journal of Physical Chemistry B, 2012, 116, 8494-8503.	1.2	276
3	Hypervalent Bonding in One, Two, and Three Dimensions: Extending the Zintl-Klemm Concept to Nonclassical Electron-Rich Networks. Angewandte Chemie - International Edition, 2000, 39, 2408-2448.	7.2	261
4	A Comparative Theoretical Study of the Hydrogen, Methyl, and Ethyl Chemisorption on the Pt(111) Surface. Journal of the American Chemical Society, 2000, 122, 4129-4144.	6.6	198
5	Role of Water Mediated Interactions in Proteinâ^'Protein Recognition Landscapes. Journal of the American Chemical Society, 2003, 125, 9170-9178.	6.6	177
6	Chemically accurate coarse graining of double-stranded DNA. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20340-20345.	3.3	150
7	Electrostatic, Steric, and Hydration Interactions Favor Na+ Condensation around DNA Compared with K+. Journal of the American Chemical Society, 2006, 128, 14506-14518.	6.6	138
8	Protein functional landscapes, dynamics, allostery: a tortuous path towards a universal theoretical framework. Quarterly Reviews of Biophysics, 2010, 43, 295-332.	2.4	131
9	Exploring the Free Energy Landscape of Nucleosomes. Journal of the American Chemical Society, 2016, 138, 8126-8133.	6.6	119
10	The physics and bioinformatics of binding and folding?an energy landscape perspective. Biopolymers, 2003, 68, 333-349.	1.2	118
11	Predictive energy landscapes for proteinâ€“protein association. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 19244-19249.	3.3	112
12	Energy Landscape Analyses of Disordered Histone Tails Reveal Special Organization of Their Conformational Dynamics. Journal of the American Chemical Society, 2011, 133, 7405-7415.	6.6	99
13	Concerted Dihedral Rotations Give Rise to Internal Friction in Unfolded Proteins. Journal of the American Chemical Society, 2014, 136, 8708-8713.	6.6	93
14	The Stochastic Dynamics of Filopodial Growth. Biophysical Journal, 2008, 94, 3839-3852.	0.2	92
15	Counterion Atmosphere and Hydration Patterns near a Nucleosome Core Particle. Journal of the American Chemical Society, 2009, 131, 15005-15013.	6.6	90
16	AWSEM-IDP: A Coarse-Grained Force Field for Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2018, 122, 11115-11125.	1.2	90
17	Regulation of the H4 tail binding and folding landscapes via Lys-16 acetylation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17857-17862.	3.3	82
18	Recent successes in coarseâ€grained modeling of DNA. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 69-83.	6.2	81

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19	MEDYAN: Mechanochemical Simulations of Contraction and Polarity Alignment in Actomyosin Networks. PLoS Computational Biology, 2016, 12, e1004877.	1.5	81
20	Molecular Renormalization Group Coarse-Graining of Polymer Chains: Application to Double-Stranded DNA. Biophysical Journal, 2009, 96, 4044-4052.	0.2	80
21	Molecular Renormalization Group Coarse-Graining of Electrolyte Solutions: Application to Aqueous NaCl and KCl. Journal of Physical Chemistry B, 2009, 113, 7785-7793.	1.2	76
22	Proteins with weakly funneled energy landscapes challenge the classical structureâ€“function paradigm. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14237-14238.	3.3	67
23	Molecular noise of capping protein binding induces macroscopic instability in filopodial dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11570-11575.	3.3	64
24	The Acetylation Landscape of the H4 Histone Tail: Disentangling the Interplay between the Specific and Cumulative Effects. Journal of the American Chemical Society, 2015, 137, 6245-6253.	6.6	64
25	Is DNAâ€™s Rigidity Dominated by Electrostatic or Nonelectrostatic Interactions?. Journal of the American Chemical Society, 2011, 133, 19290-19293.	6.6	63
26	Inter-DNA Electrostatics from Explicit Solvent Molecular Dynamics Simulations. Journal of the American Chemical Society, 2007, 129, 6060-6061.	6.6	62
27	Deconstructing the Native State: Energy Landscapes, Function, and Dynamics of Globular Proteins. Journal of Physical Chemistry B, 2009, 113, 8800-8812.	1.2	62
28	Polyelectrolytes in biology and soft matter. Soft Matter, 2012, 8, 9265.	1.2	54
29	Total energy partitioning within a one-electron formalism: A Hamilton population study of surfaceâ€“CO interaction in the c(2Â—2)-CO/ Ni(100) chemisorption system. Journal of Chemical Physics, 1999, 111, 893-910.	1.2	49
30	Interfacial Energy Conversion in Ru^{II} Polypyridyl-Derivatized Oligoproline Assemblies on TiO₂. Journal of the American Chemical Society, 2013, 135, 5250-5253.	6.6	44
31	Electron-Rich Rods as Building Blocks for Sb Strips and Te Sheets. Journal of the American Chemical Society, 2001, 123, 6600-6608.	6.6	41
32	Mechano-Chemical Feedbacks Regulate Actin Mesh Growth inÂLamellipodial Protrusions. Biophysical Journal, 2010, 98, 1375-1384.	0.2	41
33	Intrinsic elasticity of nucleosomes is encoded by histone variants and calibrated by their binding partners. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24066-24074.	3.3	41
34	Role of Topology, Nonadditivity, and Water-Mediated Interactions in Predicting the Structures of Î±/Î² Proteins. Journal of the American Chemical Society, 2006, 128, 5168-5176.	6.6	35
35	Shearing of the CENP-A dimerization interface mediates plasticity in the octameric centromeric nucleosome. Scientific Reports, 2015, 5, 17038.	1.6	35
36	Building up Complexity from Strips and Sheets: The Electronic Structure of the La12Mn2Sb30Alloy. Journal of Solid State Chemistry, 1998, 139, 8-21.	1.4	34

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37	Hierarchical organization of eglin c native state dynamics is shaped by competing direct and water-mediated interactions. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10659-10664.	3.3	33
38	Functional versus folding landscapes: the same yet different. Current Opinion in Structural Biology, 2010, 20, 16-22.	2.6	32
39	Multiscale Stochastic Reactionâ€“Diffusion Modeling: Application to Actin Dynamics in Filopodia. Bulletin of Mathematical Biology, 2014, 76, 799-818.	0.9	32
40	Remarkable structural transformations of actin bundles are driven by their initial polarity, motor activity, crosslinking, and filament treadmilling. PLoS Computational Biology, 2019, 15, e1007156.	1.5	32
41	Induced Fit, Folding, and Recognition of the NF-Î¹B-Nuclear Localization Signals by Iî¹BÎ± and Iî¹BÎ². Journal of Molecular Biology, 2007, 367, 262-274.	2.0	31
42	Theory of active transport in filopodia and stereocilia. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10849-10854.	3.3	31
43	Theoretical and computational validation of the Kuhn barrier friction mechanism in unfolded proteins. Scientific Reports, 2017, 7, 269.	1.6	31
44	Internal modifications in the CENP-A nucleosome modulate centromeric dynamics. Epigenetics and Chromatin, 2017, 10, 17.	1.8	31
45	Binding Dynamics of Disordered Linker Histone H1 with a Nucleosomal Particle. Journal of Molecular Biology, 2021, 433, 166881.	2.0	30
46	A variational approach to the stochastic aspects of cellular signal transduction. Journal of Chemical Physics, 2006, 125, 124106.	1.2	28
47	Promiscuous Histone Mis-Assembly Is Actively Prevented by Chaperones. Journal of the American Chemical Society, 2016, 138, 13207-13218.	6.6	28
48	Different translation dynamics of Î²- and Î³-actin regulates cell migration. ELife, 2021, 10, .	2.8	28
49	Stochastic Resonant Signaling in Enzyme Cascades. Physical Review Letters, 2007, 98, 228301.	2.9	27
50	Polyionic Charge Density Plays a Key Role in Differential Recognition of Mobile Ions by Biopolymers. Journal of Physical Chemistry B, 2008, 112, 9135-9145.	1.2	26
51	Computing Free Energy of a Large-Scale Allosteric Transition in Adenylate Kinase Using All Atom Explicit Solvent Simulations. Journal of Physical Chemistry B, 2012, 116, 1709-1715.	1.2	25
52	The interplay between discrete noise and nonlinear chemical kinetics in a signal amplification cascade. Journal of Chemical Physics, 2006, 125, 154901.	1.2	23
53	Probing the Configurational Space of a Metalloprotein Core:Â An ab Initio Molecular Dynamics Study of Duo Ferro 1 Binuclear Zn Cofactor. Journal of the American Chemical Society, 2003, 125, 560-569.	6.6	22
54	Energy Landscape Analysis of Protein Dimers. Israel Journal of Chemistry, 2004, 44, 281-297.	1.0	22

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55	Quantifying dissipation in actomyosin networks. Interface Focus, 2019, 9, 20180078.	1.5	21
56	Electron-Rich Bonding and the Importance of s,p Mixing as One Moves Across a Period:Â A Lesson from the LiSn System. Journal of the American Chemical Society, 2001, 123, 2317-2325.	6.6	20
57	Molecular Transport Modulates the Adaptive Response of Branched Actin Networks to an External Force. Journal of Physical Chemistry B, 2013, 117, 13388-13396.	1.2	20
58	Turnover versus treadmilling in actin network assembly and remodeling. Cytoskeleton, 2019, 76, 562-570.	1.0	20
59	Design of Active Transport Must Be Highly Intricate: A Possible Role of Myosin and Ena/VASP for G-Actin Transport in Filopodia. Biophysical Journal, 2010, 98, 1439-1448.	0.2	19
60	AWSEM-Suite: a protein structure prediction server based on template-guided, coevolutionary-enhanced optimized folding landscapes. Nucleic Acids Research, 2020, 48, W25-W30.	6.5	18
61	High Resolution Approach to the Native State Ensemble Kinetics and Thermodynamics. Biophysical Journal, 2008, 95, 5524-5532.	0.2	17
62	Tunable Energy Transfer Rates via Control of Primary, Secondary, and Tertiary Structure of a Coiled Coil Peptide Scaffold. Inorganic Chemistry, 2012, 51, 11324-11338.	1.9	17
63	The Oligomerization Landscape of Histones. Biophysical Journal, 2019, 116, 1845-1855.	0.2	17
64	Tensile force-induced cytoskeletal remodeling: Mechanics before chemistry. PLoS Computational Biology, 2020, 16, e1007693.	1.5	15
65	Membrane-MEDYAN: Simulating Deformable Vesicles Containing Complex Cytoskeletal Networks. Journal of Physical Chemistry B, 2021, 125, 10710-10719.	1.2	15
66	Generalized perturbational molecular orbital (PMO) theory. International Journal of Quantum Chemistry, 2000, 77, 408-420.	1.0	14
67	Protein fluxes along the filopodium as a framework for understanding the growth-retraction dynamics. Cell Adhesion and Migration, 2011, 5, 448-456.	1.1	14
68	Steric Effects Induce Geometric Remodeling of Actin Bundles in Filopodia. Biophysical Journal, 2016, 110, 2066-2075.	0.2	14
69	Understanding cytoskeletal avalanches using mechanical stability analysis. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	14
70	Computing free energies of protein conformations from explicit solvent simulations. Methods, 2010, 52, 115-121.	1.9	13
71	Elimination of fast variables in chemical Langevin equations. Journal of Chemical Physics, 2008, 129, 214115.	1.2	12
72	Stochastic Ratcheting on a Funneled Energy Landscape Is Necessary for Highly Efficient Contractility of Actomyosin Force Dipoles. Physical Review X, 2018, 8, .	2.8	12

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73	How does the antagonism between capping and anti-capping proteins affect actin network dynamics?. Journal of Physics Condensed Matter, 2011, 23, 374101.	0.7	11
74	Machine learning/molecular dynamic protein structure prediction approach to investigate the protein conformational ensemble. Scientific Reports, 2022, 12, .	1.6	11
75	Protein structure prediction: Do hydrogen bonding and water-mediated interactions suffice?. Methods, 2010, 52, 84-90.	1.9	10
76	Free energy calculations of counterion partitioning between DNA and chloride solutions. Mendeleev Communications, 2007, 17, 97-99.	0.6	9
77	Environmental Fluctuations and Stochastic Resonance in Protein Folding. ChemPhysChem, 2016, 17, 1341-1348.	1.0	9
78	Low-dimensional manifold of actin polymerization dynamics. New Journal of Physics, 2017, 19, 125012.	1.2	8
79	AWSEM-MD. , 2017, , 121-190.		8
80	Evolution of complex probability distributions in enzyme cascades. Journal of Theoretical Biology, 2007, 248, 537-545.	0.8	6
81	Reverse-engineering of biochemical reaction networks from spatio-temporal correlations of fluorescence fluctuations. Journal of Theoretical Biology, 2010, 264, 490-500.	0.8	6
82	Stochastic Resonance in Protein Folding Dynamics. ChemPhysChem, 2016, 17, 1305-1313.	1.0	6
83	Gibbs free energy change of a discrete chemical reaction event. Journal of Chemical Physics, 2020, 152, 084116.	1.2	6
84	Minimal Cylinder Analysis Reveals the Mechanical Properties of Oncogenic Nucleosomes. Biophysical Journal, 2020, 118, 2309-2318.	0.2	6
85	DNA Exit Ramps Are Revealed in the Binding Landscapes Obtained from Simulations in Helical Coordinates. PLoS Computational Biology, 2015, 11, e1003980.	1.5	5
86	Simulated actin reorganization mediated by motor proteins. PLoS Computational Biology, 2022, 18, e1010026.	1.5	4
87	Quantifying Dissipation in Actomyosin Networks. Biophysical Journal, 2019, 116, 254a.	0.2	3
88	Segmental Lennard-Jones interactions for semi-flexible polymer networks. Molecular Physics, 0, , e1910358.	0.8	3
89	Structural Heterogeneity and Dynamics of the Unfolded Ensemble. Israel Journal of Chemistry, 2014, 54, 1293-1301.	1.0	2
90	Nonequilibrium Water Transport in a Nonionic Microemulsion System. Journal of Physical Chemistry B, 2011, 115, 6503-6508.	1.2	1

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91	A molecular dynamics study of protein denaturation induced by sulfonate-based surfactants. Journal of Molecular Modeling, 2021, 27, 261.	0.8	1
92	Capsid Deformations Reveal Complex Mechano-Chemistry. Biophysical Journal, 2013, 105, 2233-2234.	0.2	0
93	Tensile force-induced cytoskeletal remodeling: Mechanics before chemistry. , 2020, 16, e1007693.		0
94	Tensile force-induced cytoskeletal remodeling: Mechanics before chemistry. , 2020, 16, e1007693.		0
95	Tensile force-induced cytoskeletal remodeling: Mechanics before chemistry. , 2020, 16, e1007693.		0
96	Tensile force-induced cytoskeletal remodeling: Mechanics before chemistry. , 2020, 16, e1007693.		0