# Paul Charles Whitford

List of Publications by Year
in descending order



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|---|---|---|---|
| 72 papers | 3,949 citations | 147801 31 h-index | 128289 60 g-index |
| 87 all docs | 87 docs citations | 87 times ranked | 2848 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Head swivel on the ribosome facilitates translocation by means of intra-subunit tRNA hybrid sites. Nature, 2010, 468, 713-716. | 27.8 | 336 |
| 2 | An allâ€atom structureâ€based potential for proteins: Bridging minimal models with allâ€atom empirical forcefields. Proteins: Structure, Function and Bioinformatics, 2009, 75, 430-441. | 2.6 | 327 |
| 3 | SMOG@ctbp: simplified deployment of structure-based models in GROMACS. Nucleic Acids Research, 2010, 38, W657-W661. | 14.5 | 291 |
| 4 | Conformational Transitions of Adenylate Kinase: Switching by Cracking. Journal of Molecular Biology, 2007, 366, 1661-1671. | 4.2 | 272 |
| 5 | SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLoS Computational Biology, 2016, 12, e1004794. | 3.2 | 226 |
| 6 | Nanopore-Based Measurements of Protein Size, Fluctuations, and Conformational Changes. ACS Nano, 2017, 11, 5706-5716. | 14.6 | 219 |
| 7 | The Shadow Map: A General Contact Definition for Capturing the Dynamics of Biomolecular Folding and Function. Journal of Physical Chemistry B, 2012, 116, 8692-8702. | 2.6 | 189 |
| 8 | Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. Rna, 2010, 16, 1196-1204. | 3.5 | 174 |
| 9 | Biomolecular dynamics: orderâ€“disorder transitions and energy landscapes. Reports on Progress in Physics, 2012, 75, 076601. | 20.1 | 105 |
| 10 | Conformational Transitions in Adenylate Kinase. Journal of Biological Chemistry, 2008, 283, 2042-2048. | 3.4 | 95 |
| 11 | Nonlocal Helix Formation Is Key to Understanding S-Adenosylmethionine-1 Riboswitch Function. Biophysical Journal, 2009, 96, L7-L9. | 0.5 | 95 |
| 12 | Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. Journal of the American Chemical Society, 2012, 134, 12043-12053. | 13.7 | 91 |
| 13 | Excited states of ribosome translocation revealed through integrative molecular modeling. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 18943-18948. | 7.1 | 89 |
| 14 | Extracting function from a Î²-trefoil folding motif. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10384-10389. | 7.1 | 79 |
| 15 | Connecting the Kinetics and Energy Landscape of tRNA Translocation on the Ribosome. PLoS Computational Biology, 2013, 9, e1003003. | 3.2 | 79 |
| 16 | Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Physical Review Letters, 2015, 114, 258105. | 7.8 | 69 |
| 17 | Topography of funneled landscapes determines the thermodynamics and kinetics of protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15763-15768. | 7.1 | 62 |
| 18 | Energy landscape along an enzymatic reaction trajectory: Hinges or cracks?. HFSP Journal, 2008, 2, 61-64. | 2.5 | 60 |

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|---|---|---|---|
| 19 | How EF-Tu can contribute to efficient proofreading of aa-tRNA by the ribosome. Nature Communications, 2016, 7, 13314. | 12.8 | 57 |
| 20 | Mutations as trapdoors to two competing native conformations of the Rop-dimer. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 17674-17679. | 7.1 | 53 |
| 21 | A Novel Disulfide Bond in the SH2 Domain of the C-terminal Src Kinase Controls Catalytic Activity. Journal of Molecular Biology, 2007, 365, 1460-1468. | 4.2 | 52 |
| 22 | Steric interactions lead to collective tilting motion in the ribosome during mRNAâ€“tRNA translocation. Nature Communications, 2016, 7, 10586. | 12.8 | 52 |
| 23 | Connecting Energy Landscapes with Experimental Rates for Aminoacyl-tRNA Accommodation in the Ribosome. Journal of the American Chemical Society, 2010, 132, 13170-13171. | 13.7 | 48 |
| 24 | Order and disorder control the functional rearrangement of influenza hemagglutinin. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 12049-12054. | 7.1 | 47 |
| 25 | Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophysical Journal, 2014, 106, 1508-1519. | 0.5 | 46 |
| 26 | Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome. Biophysical Journal, 2014, 107, 2881-2890. | 0.5 | 44 |
| 27 | Consensus among flexible fitting approaches improves the interpretation of cryo-EM data. Journal of Structural Biology, 2012, 177, 561-570. | 2.8 | 38 |
| 28 | Coordinate and time-dependent diffusion dynamics in protein folding. Methods, 2010, 52, 91-98. | 3.8 | 36 |
| 29 | Design and proof of concept for targeted phage-based COVID-19 vaccination strategies with a streamlined cold-free supply chain. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 7.1 | 35 |
| 30 | The Origin of Nonmonotonic Complex Behavior and the Effects of Nonnative Interactions on the Diffusive Properties of Protein Folding. Biophysical Journal, 2010, 99, 600-608. | 0.5 | 33 |
| 31 | Proteins at Work. Journal of Biological Chemistry, 2010, 285, 36121-36128. | 3.4 | 32 |
| 32 | Diffusion of tRNA inside the ribosome is position-dependent. Journal of Chemical Physics, 2019, 151, 085102. | 3.0 | 31 |
| 33 | What protein folding teaches us about biological function and molecular machines. Current Opinion in Structural Biology, 2015, 30, 57-62. | 5.7 | 30 |
| 34 | Simulating movement of tRNA through the ribosome during hybrid-state formation. Journal of Chemical Physics, 2013, 139, 121919. | 3.0 | 29 |
| 35 | Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. ELife, 2021, 10, . | 6.0 | 29 |
| 36 | Structural insights into mRNA reading frame regulation by tRNA modification and slippery codonâ€“anticodon pairing. ELife, 2020, 9, . | 6.0 | 28 |

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|---|---|---|---|
| 37 | Allostery in the ferredoxin protein motif does not involve a conformational switch. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 2240-2245. | 7.1 | 27 |
| 38 | Distinguishing Biomolecular Pathways and Metastable States. Journal of Chemical Theory and Computation, 2019, 15, 6482-6490. | 5.3 | 23 |
| 39 | Anisotropic Fluctuations in the Ribosome Determine tRNA Kinetics. Journal of Physical Chemistry B, 2017, 121, 10593-10601. | 2.6 | 21 |
| 40 | Studying ribosome dynamics with simplified models. Methods, 2019, 162-163, 128-140. | 3.8 | 21 |
| 41 | Exploring the Balance between Folding and Functional Dynamics in Proteins and RNA. International Journal of Molecular Sciences, 2015, 16, 6868-6889. | 4.1 | 20 |
| 42 | How the Ribosomal A-Site Finger Can Lead to tRNA Species-Dependent Dynamics. Journal of Physical Chemistry B, 2017, 121, 2767-2775. | 2.6 | 20 |
| 43 | Disorder guides domain rearrangement in elongation factor Tu. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1037-1046. | 2.6 | 16 |
| 44 | Quantifying the Relationship between Single-Molecule Probes and Subunit Rotation in the Ribosome. Biophysical Journal, 2017, 113, 2777-2786. | 0.5 | 15 |
| 45 | Dissecting the Energetics of Subunit Rotation in the Ribosome. Journal of Physical Chemistry B, 2019, 123, 2812-2823. | 2.6 | 15 |
| 46 | Substrate-Specific Reorganization of the Conformational Ensemble of CSK Implicates Novel Modes of Kinase Function. PLoS Computational Biology, 2012, 8, e1002695. | 3.2 | 14 |
| 47 | Disorder guides protein function. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 7114-7115. | 7.1 | 14 |
| 48 | Drift-diffusion (DrDiff) framework determines kinetics and thermodynamics of two-state folding trajectory and tunes diffusion models. Journal of Chemical Physics, 2019, 151, 114106. | 3.0 | 14 |
| 49 | Capturing Transition States for tRNA Hybrid-State Formation in the Ribosome. Journal of Physical Chemistry B, 2016, 120, 8768-8775. | 2.6 | 13 |
| 50 | A steric gate controls P/E hybrid-state formation of tRNA on the ribosome. Nature Communications, 2020, 11, 5706. | 12.8 | 13 |
| 51 | Simulations of Phage T7 Capsid Expansion Reveal the Role of Molecular Sterics on Dynamics. Viruses, 2020, 12, 1273. | 3.3 | 13 |
| 52 | How Nanopore Translocation Experiments Can Measure RNA Unfolding. Biophysical Journal, 2020, 118, 1612-1620. | 0.5 | 13 |
| 53 | <scp>SMOG 2 and OpenSMOG: Extending the</scp> limits of structureâ€based models. Protein Science, 2022, 31, 158-172. | 7.6 | 11 |
| 54 | The Dynamics of Subunit Rotation in a Eukaryotic Ribosome. Biophysica, 2021, 1, 204-221. | 1.4 | 10 |

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| 55 | Diffuse Ions Coordinate Dynamics in a Ribonucleoprotein Assembly. Journal of the American Chemical Society, 2022, 144, 9510-9522. | 13.7 | 10 |
| 56 | Genetic and Structural Analysis of SARS-CoV-2 Spike Protein for Universal Epitope Selection. Molecular Biology and Evolution, 2022, 39, . | 8.9 | 7 |
| 57 | Massive conformation change in the prion protein: Using dualâ€basin structureâ€based models to find misfolding pathways. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1299-1307. | 2.6 | 6 |
| 58 | The ribosomeâ€™s energy landscape: Recent insights from computation. Biophysical Reviews, 2015, 7, 301-310. | 3.2 | 6 |
| 59 | pH and the Breast Cancer Recurrent Mutation D538G Affect the Process of Activation of Estrogen Receptor Î±. Biochemistry, 2022, 61, 455-463. | 2.5 | 5 |
| 60 | Enhanced septahedral ordering in cold Lennard-Jones fluids. Physical Review E, 2005, 72, 021203. | 2.1 | 4 |
| 61 | Challenges in describing ribosome dynamics. Physical Biology, 2017, 14, 023001. | 1.8 | 4 |
| 62 | Probing remote residues important for catalysis in Escherichia coli ornithine transcarbamoylase. PLoS ONE, 2020, 15, e0228487. | 2.5 | 4 |
| 63 | Extended-range order, diverging static length scales, and local structure formation in cold Lennard-Jones fluids. Journal of Chemical Physics, 2005, 122, 044508. | 3.0 | 3 |
| 64 | How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. Israel Journal of Chemistry, 2014, 54, 1093-1107. | 2.3 | 3 |
| 65 | Using SMOG 2 to Simulate Complex Biomolecular Assemblies. Methods in Molecular Biology, 2019, 2022, 129-151. | 0.9 | 3 |
| 66 | Molecular Dynamics Simulations of the Ribosome. , 2012, , 51-68. | | 2 |
| 67 | The energetics of subunit rotation in the ribosome. Biophysical Reviews, 2021, 13, 1029-1037. | 3.2 | 2 |
| 68 | Overview of the Biomolecular Association and Dynamics session at the 20th IUPAB congress, 45th Brazilian congress of SBBF, and the 50th annual meeting of SBBq. Biophysical Reviews, 2021, 13, 863-865. | 3.2 | 1 |
| 69 | Quantifying biomolecular diffusion with a â€œspherical cowâ€•model. American Journal of Physics, 2022, 90, 225-238. | 0.7 | 1 |
| 70 | Information Processing by Nanomachines: Decoding by the Ribosome. , 2011, , 67-86. | | 0 |
| 71 | Cover Image, Volume 86, Issue 10. Proteins: Structure, Function and Bioinformatics, 2018, 86, C1-C1. | 2.6 | 0 |
| 72 | Experimental and computational techniques for studying structural dynamics and function of RNA. Methods, 2019, 162-163, 1-2. | 3.8 | 0 |