Curriculum Vitae: Paul C. Whitford

Northeastern University
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Current Position

2018- Associate Professor
Department of Physics
Northeastern University, Boston, MA

2012-2018 Assistant Professor
Department of Physics
Northeastern University, Boston, MA

Education

2003-2009 **University of California at San Diego, San Diego, CA**
Advisor: José N. Onuchic
Ph.D. Physics (Biophysics): Conferred 6/13/2009

2000-2003 **Worcester Polytechnic Institute**
Bachelor of Science in Physics with *High Distinction*
Minor in Mathematics

Research Positions

2012-current **Scientific Computing Liaison to Brazil**
Rice University

2012 **Research Coordinator for High Performance Computing/ Senior Scientist**
Rice University
Center for Theoretical Biological Physics

2009-2012 **Director's Postdoctoral Fellow**
Los Alamos National Laboratory, Los Alamos, NM
Sponsor: Karissa Sanbonmatsu

2003-2009 **Graduate Researcher**
University of California, San Diego, CA

2002-2003 **Research Assistant and Undergraduate Thesis Research**
Computational investigation of glass-forming liquids
Worcester Polytechnic Institute, Worcester, MA

2001 **Research Assistant**
Light scattering spectroscopy of complex fluids
Worcester Polytechnic Institute, Worcester, MA

Honors and Awards

2014-2018 *NSF CAREER Award*

2009 *Director's Postdoctoral Fellowship*
Los Alamos National Laboratory

2009 *Funded Visits for Outstanding Students Award*
Weizmann Institute of Science, Israel

2004-2009 *Center for Theoretical Biological Physics Fellow*
University of California at San Diego

2007	*International ICAM Junior Exchange Award* Funded collaboration with scientists in São Paulo, Brazil
2005-2007	*Molecular Biophysics Training Grant Fellow* University of California at San Diego
2003-2005	*San Diego Fellowship* Office of Graduate Studies, University of California at San Diego
2003	*SPS Leadership Scholarship* Awarded by the Society of Physics Students national organization
2003	*Dr. Robert H. Goddard Award* for outstanding performance in research Faculty of Physics, Worcester Polytechnic Institute, Worcester, MA
2002	Inducted into *Tau Beta Pi*: National Engineering Honor Society
2002	Inducted into *Pi Mu Epsilon*: National Mathematics Honor Society
2002	Inducted into *Sigma Pi Sigma*: National Physics Honor Society

Talks

[83] Protein Folding on the Ribosome. May 2, 2022. *Invited.*

[82] Center for Nonlinear Studies, Los Alamos National Laboratory. April 20, 2022.

[81] *Protein Society Special Tools Issue 2022* Webinar. April 14th, 2022. Invited

[80] Weill Cornell Medine Graduate School Biophysics Research Seminar. March 20, 2022.

[79] Florida State University, Institute of Molecular Biophysics Seminar. March 8, 2022.

[78] AMD HPC Users Forum. Virtual meeting. *September 28, 2021. Invited.*

[77] AMD HPC Fund Tech Talk. Virtual meeting. *July 23, 2021. Invited.*

[76] Phage/Virus Assembly 2021. Virtual meeting. *July 28, 2021. selected*

[75] Brazilian Biophysical Society. Virtual meeting. June 21, 2021. *Invited.*

[74] 64th Annual Meeting of the Biophysical Society. San Diego, CA. *February 18th, 2020*. *Invited.*

[73] Greater Boston Area Statistical Mechanics Meeting. Brandeis University. Waltham, MA. *October 19th, 2019.*

[72] Physical Chemistry Seminar. Boston College. Chestnut Hill, MA. *September 6th, 2019.*

[71] Biomolecules and Nanostructures 7. Gdansk, Poland. *May 18th, 2019. Invited.*

[70] Nuclear and Cytoplasmic Molecular Machines at Work. NYU Abu Dhabi. Abu Dhabi, United Arab Emirates. *April 9th, 2019. Invited.*

[69] American Physical Society March Meeting. Boston, MA. *March 8th, 2019.*

[68] Massachusetts Structural Biology Club. UMass Medical School. Worcester, MA. *November 6th, 2018.*

[67] Northeast Cyberteam Conference. Worcester Polytechnic Institute, Worcester, MA. *October 19th, 2018. Plenary.*

[66] 32nd Gibbs Biothermodynamics Conference. Carbondale, IL. *October 9th, 2018. Invited.*

[65] XXVIII Congresso da Sociedade Brasileira Biofisica. Santos, Brasil. *September 29th, 2018. Invited.*

[64] 2nd Sympsosium on Current Topics in Molecular Biophysics. Santos, Brasil. *September 26th, 2018. Invited.*

[63] 32nd Symposium of The Protein Society. Boston, MA. *July 10th, 2018.*

[62] CTBP Colloquium. Rice University. *March 6th, 2018.*

[61] Physics Seminar. University at Buffalo. *February 27th, 2018.*

[60] Moderna Therapeutics Seminar. Cambridge, MA. *December 11th, 2017.*

[59] MRSEC Seminar. Brandeis University. Waltham, MA. *December 7th, 2017.*

[58] Congresso da Sociedade Brasileira de Biofísica. Santos, Brazil. *October 28th, 2017. Invited.*

[57] Physics and Biology of Proteins. International Institute of Physics. Natal, Brazil. *June 21st, 2017. Invited.*

[56] Squishy Physics Seminar. Harvard University, Cambridge, MA. *April 19th, 2017.*

[55] Physical Chemistry Seminar. University of California, San Diego, CA. *November 1st, 2016.*

[54] Biochemistry and Biophysics Seminar. University of Rochester Medical School. Rochester, NY. *September 29th, 2016.*

[53] Center for Nonlinear Studies Annual Conference. Santa Fe, NM. *May 12th, 2016. Invited.*

[52] Chemical Engineering Colloquium. University of New Hampshire. Durham, NH. *April 29th, 2016.*

[51] Biophysics Seminar. Rensselaer Polytechnic Institute. Troy, NY. *April 25th, 2016.*

[50] Biophysical Society National Meeting. Los Angeles, CA. *March 1st, 2016. Selected*.

[49] NSF Workshop: Modeling and Dynamics in Molecular Biophysics. Arlington, VA. *January 27th, 2016. Invited.*

[48] Gordon Research Conference, Protein Folding Dynamics. Galveston, TX. *January, 11th, 2016. Invited.*

[47] Multiscale Motility of Biomolecular Machines. Max Planck Institute. Berlin, Germany. *December 9th, 2015. Invited.*

[46] Biophysics Seminar. University of Maryland, College Park. *October 19th, 2015.*

[45] Simon's Lecture. National Centre for Biological Sciences. Bangalore, India. *July 14th, 2015.*

[44] Albany 2015: Conversation 19. SUNY Albany. Albany, NY. *June 11th, 2015. Young Scientist Lecture.*

[43] Physics Department Colloquium. Worcester Polytechnic Institute. Worcester, MA. *March 30th, 2015.*

[42] Workshop em Biofísica Molecular. Universidade Estadual Paulista. São José do Rio Preto, SP, Brazil. *January 9th, 2015. Plenary Lecture.*

[41] Physical Chemistry Seminar. Department of Chemistry. Boston University. Boston, MA. *October 29th, 2014.*

[40] Significance of Knotted Structures for Function of Proteins and Nucleic Acids. University of Warsaw. Warsaw, Poland. *September 19th, 2014. Invited.*

[39] RiboCORE Seminar Series. Uppsala University. Uppsala, Sweden. *September 11th, 2014.*

[38] 1st Symposium on Current Topics in Molecular Biophysics. São Paulo, Brazil. *May 22nd 2014.*

[37] Fassberg Seminar Series. Max Planck Institute of Biophysical Chemistry. Gottingen, Germany. *February 11th, 2014.*

[36] Max Planck Institute of Colloids and Interfaces. Potsdam, Germany. *February 6th, 2014.*

[35] 552nd WE Heraeus Seminar – Physics of Biomolecular Folding and Assembly: Theory meets experiment. Bad Honnef, Germany. *February 5th, 2014. Invited.*

[34] 1st Annual Sigma-Aldrich Symposium on RNA Science and its Applications. SUNY Albany, Albany, NY. *January, 23rd, 2014. Selected.*

[33] University of New England. Department of Pharmaceutical Sciences. Portland, ME. *October 15th, 2013.*

[32] University of Rhode Island. Chemistry Department Colloquium. Kingston, RI. *September 23rd, 2013.*

[31] 27th Protein Society Symposium. Boston, MA. *July 23rd, 2013. Young Investigator Speaker.*

[30] Albany 2013: Conversation 18. SUNY Albany. Albany, NY. *June 12th, 2013. Young Scientist Lecture.*

[29] 12th Chemical Biophysics Symposium. University of Toronto. Toronto, Ontario. *April 20th, 2013. Invited Keynote Speaker*

[28] Northeastern University. Biology Department Colloquium. Boston, MA. *January, 28th, 2013.*

[27] Integra o Centro de Pesquisa em Energia e Materiais (CNPEM). Laboratório Nacional de Ciência e Tecnologia do Bioetanol. Campinas, SP, Brazil. *December 13th, 2012.*

[26] Universidade de São Paulo. Instituto de Química. São Paulo, SP, Brazil. *August 10th, 2012.*

[25] Universidade Estadual Paulista. Department of Physics. São José do Rio Preto, SP, Brazil. *May 29th, 2012.*

[24] State University of New York at Albany. Department of Chemistry. Albany, NY. *March 7th, 2012.*

[23] Biophysical Society 56th Annual Meeting. San Diego, CA. *February 26th, 2012. Selected.*

[22] Hospital for Sick Children. Molecular Structure and Function Program seminar series. Toronto, Canada. *October 24th, 2011.*

[21] 1st KIAS Conference on Subcellular Dynamics. Seoul, South Korea. *July 26th, 2011. Invited*

[20] International Conference on Biological Physics Workshop. San Diego, CA. *June 21st, 2011. Invited*

[19] University of Rochester Medical Center. Department of Biochemistry and Biophysics. Rochester, NY. *March 10th, 2011.*

[18] College of Staten Island. Department of Chemistry. New York, NY. *November 18th, 2010.*

[17] State University of New York at Stony Brook. Department of Chemistry. Stony Brook, NY. *November 15th, 2010.*

[16] City College of New York. Department of Physics. New York, NY. *November 10th, 2010.*

[15] Hebrew University in Jerusalem. The Alexander Silberman Institute of Life Sciences. Jerusalem, Israel. *August 16th, 2010.*

[14] Weizmann Institute of Science. Department of Structural Biology. Rehovot, Israel. *July 21st, 2010.*

[13] TSRI Characterizing Energy Landscapes Workshop. Telluride, CO. *June 15th, 2010. Invited*

[12] University of Potsdam. Institute of Biochemistry and Biology. Potsdam, Germany. *April 29th, 2010.*

[11] Charité Universitätsmedizin Berlin. Institut Für Medizinische Physik und Biophysik. Berlin, Germany. *February 15th, 2010.*

[10] Max Planck Institute for Biophysical Chemistry. Department of Theoretical and Computational Chemistry. Göttingen, Germany. *February 10th, 2010.*

[9] 23rd tRNA Workshop. Aveiro, Portugal. *February 1st, 2010. Selected*

[8] University of California at Santa Cruz. Department of Molecular, Cellular and Developmental Biology. Santa Cruz, CA. *September 21st, 2009.*

[7] RNA Society 14th Annual Meeting. Madison, Wisconsin, *May 28th, 2009. Selected*

[6] Guest Lecture. CSU San Marcos. Department of Physics. San Marcos, CA. *March 16th, 2009.*

[5] Weill Medical College of Cornell University. Department of Physiology and Biophysics. New York, NY. *March 9th, 2009.*

[4] Rensselaer Polytechnic Institute. Department of Physics. Troy, NY. *March 5th, 2009*.

[3] Biophysical Society 53rd Annual Meeting. Boston, MA. *March 4th, 2009. Selected*

[2] Universidade Estadual Paulista. Department of Physics. São José do Rio Preto, SP, Brazil. *September 27th, 2007.*

[1] TSRI Energy Landscapes Workshop. Telluride, CO. *April 4th, 2007. Invited*

Reviewer Activity

Hundreds of manuscripts and multiple books for over 60 journals and publishers.

Reviewer and panelist for various US-based and international science and computing agencies.

Editorial Roles

2022 Guest editor for JPC Festschrift (Jose Onuchic)
2021- *Frontiers in Chemistry,* Associate Editor
2021- *Frontiers in Physics,* Associate Editor
2021- *Biophysica*, Editorial Board Member

2019 Guest co-editor for special issue of *Methods* "Experimental and computational techniques for studying structural dynamics and function of RNA"

Current Grants

9/1/20-8/30/25: *Center for Theoretical Biological Physics.* NSF Physics Frontier Center Program. $12,900,000 (Role: Senior Investigator)

7/1/19-6/30/23: *Quantifying the effects of ions and collective rearrangements during ribosome function. NSF-MCB* $797,314 (Role: PI)

Completed Grant

1/1/14-12/31/19: CAREER: Disorder, tRNA composition and energy transduction in the ribosome. *NSF-MCB* $956,688 (Role: PI)

Awarded Computing Allocations

1/1/13-12/31/13: XSEDE Computing Award for "Using High Performance Computing to Reveal the Functional Dynamics of the Ribosome." 2.0 million Service Units on the Kraken and Stampede clusters. Role: PI.

1/1/11-12/31/11: TeraGrid Computing Award for "Using High Performance Computing to Reveal the Functional Dynamics of the Ribosome." 4.1 million Service Units on the AQS, Trestles and Lonestar clusters. Role: PI.

Professional Affiliations

2012-current RNA Institute at SUNY Albany: External Faculty Affiliate.

2013-current Center for Theoretical Biological Physics: Senior Investigator.

Teaching, Mentoring and Professional Activities

Courses: PHYS1165: Physics 2 (Undergraduate Electricity and Magnetism)
PHYS4305: Thermodynamics and Statistical Mechanics (Undergraduate)
PHYS7301: Classical Mechanics/Mathematical Methods (Graduate)
PHYS7321: Computational Physics (Graduate)
PHYS7305: Statistical Physics (Graduate)

October 2022 **Module Leader** Training program in quantitative biology and ecology. Serrapilheira Institute and ICTP-SAIFR. University of São Paulo, Brazil.

Summer 2022 **Lead Organizer** Workshop: Simulating ribosomes, chromosomes and other large assemblies (scheduled).

Oct. 2023 **Organizer** 3rd *Symposium on Current Topics in Molecular Biophysics.* São Paulo, Brazil (anticipated).

3/18/2020 **Co-Organizer** RNAsim 2020 mini-symposium. SUNY Albany. (Cancelled, due to COVID)

11/9/2019 **Lead Organizer** Molecular Biophysics in the Northeast (MBN) 2019. Northeastern University.

3/21/2019 **Organizer and Presenter** *RNA Dynamics: Structure Prediction and Dynamics.* RNA Institute, SUNY Albany, Albany, NY.

9/24-27/2018 **Organizer** *2nd Symposium on Current Topics in Molecular Biophysics.* Santos, Brazil.

3/15/2018 **Organizer and Presenter** *RNA Dynamics: Multiscale simulations of RNA.* RNA Institute, SUNY Albany, Albany, NY.

2/13&20/18 **Organizer and Presenter** *Exploring Molecular Biophysics Through Computing.* Workshop for high school students, in collaboration with

Holyoke Codes and The Urban League of Springfield. Springfield and Holyoke, MA.

1/5-6/18 **Organizer** *Symposium in Celebration of José Onuchic's 60th Birthday.* Rice University. Houston, TX.

6/21-23/2017 **Presenter** *Introduction to structure-based models.* International Institute of Physics. Natal, Brazil.

3/16/2017 **Organizer** *RNA Dynamics: Interpretation of experiments through simulation*. RNA Institute, SUNY Albany, Albany, NY.

10/17/2016 **Workshop Organizer and Presenter** *4° Workshop de High Performance Computing – Convênio: USP – Rice University*. University of São Paulo, São Paulo, SP, Brazil.

3/17/2016 **Organizer** *RNA Dynamics: Molecular modeling through simulation*. RNA Institute, SUNY Albany, Albany, NY.

4/17/2015 **Workshop Organizer and Presenter** *3° Workshop de High Performance Computing – Convênio: USP – Rice University*. University of São Paulo, São Paulo, SP, Brazil.

4/11/2015 **Co-organizer** *New England Undergraduate Computing Symposium 2015*. Boston University, Boston, MA.

3/19/2015 **Organizer** *RNA Dynamics: Going from In Vitro to In Silico*. RNA Institute, SUNY Albany, Albany, NY.

5/21-23/2014 **Organizer** *1st Symposium on Current Topics in Molecular Biophysics.* University of São Paulo, São Paulo, Brazil.

4/14/2014 **Workshop Organizer and Presenter** *2° Workshop de High Performance Computing – Convênio: USP – Rice University*. University of São Paulo, São Paulo, SP, Brazil.

3/29/2014 **Co-organizer** *New England Undergraduate Computing Symposium 2014*. Boston University, Boston, MA.

12/6-7/2012 **Workshop Organizer and Presenter** *Status e Operações do Supercomputador USP-Rice Blue Gene/P*. University of São Paulo, São Paulo, SP, Brazil.

May 2007 **Principal Organizer and Presenter** CTBP-Workshop on Protein Dynamics, *Models, Simulations and Thermodynamics* workshop for graduate students

2006 **Mentor** of Research Experience for Undergraduate (REU) student.

2004 **Organizer and Presenter:** "Physics Majors Users Guide (PMUG)" Department of Physics, University of California at San Diego

2003-2005 **Participant** Preparing Future Physics Faculty Program Department of Physics, University of California at San Diego

2001-2003 **Peer Learning Assistant (Undergraduate TA)**
Department of Mathematics
Worcester Polytechnic Institute, Worcester, MA

Service

2021 Massachusetts Green High Performance Computing Center (MGHPCC) Steering Committee

2017-current *Information Technology Policy Committee*

2017-current *College of Science College Council* (Chair, 2018-2020)

2012-current *NU Research Computing Committee*

Responsible for advising university activities at the Massachusetts Green High Performance Computing Center
Committee Chair (2016-current)

2016-2019 *Physics Department Graduate Committee*

2012-2017 *Physics Department Colloquium Committee*

2003-2006 *UCSD Graduate Student Association*
Vice-president of External Affairs in 2004-2005
Graduate representative to the state and federal legislature
State-level activities: Coordinated and participated in lobbying and testimonies before state legislators. Focused on bills that would improve accessibility, affordability, equality and academic integrity at UC.

Federal-level activities: Coordinated and participated in lobbying congress members and federal agencies. Focused on advocating for improved international student support and federal financial aid programs.

2004-2005 *University of California Student Association*
Chair of Graduate and Professional Student Committee
Graduate representative to the state and federal legislature and UCOP

2004-2005 *Science Policy Analysis Roundtable*
Co-organizer and participant
Activities included journal club-like seminars with graduate student, post-doctoral, faculty and invited speakers from across California. Topics included ethics in science and academia, societal impacts of science, science policy and other contemporary issues.

2004-2009 *UCSD Academic Integrity Hearing Board*
Board Member

2000-2003 *Society of Physics Students*
President for 2002-2003 of Worcester Polytechnic Institute Chapter
Member of National Council, representing New England for 2002-03
Principal organizer of New England Zone meeting

Publications (* corresponding author; 75 publications)

Research Articles

[56] A. Wang, M. Levi, U. Mohanty*, P. C. Whitford*. Diffuse ions coordinate dynamics in a ribonucleoprotein assembly. *Journal of the American Chemical Society.* 2022.

[55] C. Markosian, D. I. Staquicini, P. Droga, E. Dodero-Rojas, J. H. Lubin, F. H. F. Tang, T. L. Smith, V. G. Contessoto, S. K. Libutti, Z. Wang, V. Cristini, S. D. Khare, P. C. Whitford, S. K. Burley, J. N. Onuchic, R. Pasqualini, W. Arap. Genetic and structural analysis of SARS-CoV-2 spike protein for universal epitope selection. *Molecular Biology & Evolution.* **39**, msac091, 2022.

[54] V. M. Oliveira, M. M. G. Dias, T. M. Avelino, N. B. Videira, F. B. da Silva, T. R. Doratioto, P. C. Whitford, V. B. P. Leite, A. C. M. Figueira. pH and the breast cancer recurrent mutation D538G affect the process of activation of Estrogen Receptor alpha. *Biochemistry,* **61**, 455-463, 2022.

[53] A. B. Oliveira Jr, V. G. Contessoto, A. Hassan, S. Byju, A. Wang, Y. Wang, E. Dodero-Rojas, U. Mohanty, J. K. Noel*, J. N. Onuchic*, P. C. Whitford*. SMOG2 and OpenSMOG: Extending the limits of structure-based models. *Protein Science*, **31**, 158-172, 2022.

[52] F. C. Freitas, G. Fuchs, R. J. De Oliveira, P. C. Whitford* The dynamics of subunit rotation in a eukaryotic ribosome. *Biophysica,* **1**, 204-221, 2021

[51] D. I. Staquicini, F. H.F. Tang, C. Markosian, V. J. Yao, F. I. Staquicini, E. Dodero-Rojas, V. G. Contessoto, D. Davis, P. O'Brien, N. Habib, T. L. Smith, N. Bruiners, R. L. Sidman, M. L. Gennaro, E. C. Lattime, S. K. Libutti, P. C. Whitford, S. K. Burley, J. N. Onuchic, W. Arap, R. Pasqualini. Design and proof-of-concept for targeted phage-based COVID-19 vaccination strategies with a streamlines cold-free supply chain. *PNAS* **118**, e2105739118, 2021.

[50] E. Dodero-Rojas, J. N. Onuchic*, P. C. Whitford* Sterically-confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. *eLife,* **10**, e70362, 2021.

[49] M. Levi, K. Walak, A. Wang, U. Mohanty, P. C. Whitford* A steric gate controls P/E hybrid-state formation of tRNA on the ribosome. *Nature Communications.* **11**, 5706, 2020.

[48] P. C. Whitford*, W. Jiang, P. Serwer. Simulations of phase T7 capsid expansion reveal the role of molecular steric on dynamics. *Viruses.* **12**, 1273, 2020.

[47] E. Hoffer, S. Hong, S. Sunita, T. Maehigashi, R.L. Gonzalez Jr, P. Whitford, C.M. Dunham. Structural insights into mRNA reading frame regulation by tRNA modification and slippery codon-anticodon pairing. eLife, **9,** e51898, 2020.

[46] L. Ngu, J. N. Winters, K. Nguyen, K. E. Ramos, N. A. DeLateur, L. Makowski, P. C. Whitford, M. J. Ondrechen, P. J. Beuning. Probing remote residues important for catalysis in *Escherichia coli* Ornithine Transcarbamoylase. *PLOS ONE.* 2020

[45] P. Bandarkar, H. Yang, R. Y. Henley, M. Wanunu*, P. C. Whitford* How nanopore experiments can measure RNA unfolding. *Biophysical Journal.* 2020

[44] H. Yang, P. Bandarkar, R. Horne, J. Chahine, V.B.P Leite, P. C. Whitford*. Diffusion of tRNA inside of the ribosome is position-dependent. *J. Chem. Phys.* 2019. (Feature Article; 2019 Editor's Choice)

[43] A. B. Oliveira Jr, H. Yang, P. C. Whitford, V. B. P Leite. Distinguishing Biomolecular Pathways and Metastable States *J. Chem. Theory Comp.* 2019.

[42] F. C. Freitas, A. N. Lima, V. G. Contessoto, P. C. Whitford, R. J. Oliveira. Drift-diffusion framework determines kinetics and thermodynamics of two-state folding trajectories and tunes diffusion models. *J. Chem. Phys.* 2019.

[41] M. Levi, P. C. Whitford*. Dissecting the energetics of subunit rotation in the ribosome. *J. Phys. Chem. B* **123**, 2812-2823, 2019.

[40] H. Yang, J. Perrier, P. C. Whitford*. Disorder guides domain rearrangement in EF-Tu. *Proteins: Structure, Function, Bioinformatics.* **86**, 1037-1046, 2018. (Cover article)

[39] M. Levi, K. Nguyen, L. Dukaye, P. C. Whitford*. Quantifying coupling between single-molecule measures and subunit rotation in the ribosome. *Biophys. J.* **113**, 2777-2786, 2017.

[38] H. Yang, J. K. Noel, P.C. Whitford*. Anisotropic fluctuations in the ribosome determine tRNA kinetics. *J. Phys. Chem. B*. **121**, 10593-10601, 2017. (Cover article)

[37] P. Waduge, R. Hu, P. Bandarkar, H. Yamazaki, B. Cressiot, Q. Zhao, P. C. Whitford*, M. Wanunu*. Nanopore-based measurements of protein size, fluctuations, and conformational changes. *ACS Nano*. **11**, 5706-5716, 2017.

[36] K. Nguyen, H. Yang, P. C. Whitford*. How the ribosomal A-site finger can lead to tRNA species-dependent dynamics. *J. Phys. Chem. B* **121**, 2767-2775, 2017.

[35] J. K. Noel, P. C. Whitford*. How EF-Tu can contribute to efficient proofreading of aa-tRNA by the ribosome. *Nature Communications* **7**, 13314, 2016.

[34] K. Nguyen, P. C. Whitford*. Capturing transition states for tRNA hybrid-state formation in the ribosome. *J. Phys. Chem. B.* **120**, 8768-8775, 2016.

[33] J. K. Noel*, M. Levi, M. Raghunathan, H. Lammert, R. L. Hayes, J. N. Onuchic*, P. C. Whitford*. SMOG 2: A versatile software package for generating structure-based models. *PLoS Comp. Biol*. **12**, e1004794, 2016.

[32] K. Nguyen, P. C. Whitford*. Steric interactions lead to collective head tilting during mRNA-tRNA translocation on the ribosome. *Nature Communications.* **7**, 10586, 2016.

[31] R. Hayes, J. K. Noel, A. Mandic, P. C. Whitford, K. Y. Sanbonmatsu, U. Mohanty, J. N. Onuchic. Generalized manning condensation model captures the RNA ion atmosphere. *Phys. Rev. Lett.* **114**, 258105, 2015.

[30] J. Jackson, K. Nguyen, P. C. Whitford*. Exploring the balance between folding and function in proteins and RNA. *Int. J. Mol. Sci.* **16***,* 6868-6889, 2015.

[29] J. K. Noel, J. Chahine, V. B. P. Leite, P. C. Whitford*. Capturing transition paths and transition states for conformational rearrangements in the ribosome. *Biophys. J.* **107**, 2872-2881, 2014.

[28] X. Lin, N. R. Eddy, J. K. Noel, P. C. Whitford, Q. Wang, J. Ma, J. N. Onuchic. Order and disorder control the functional rearrangement of influenza hemagglutinin. *Proc. Nat. Acad. Sci. USA*. **111**, 12049-12054, 2014.

[27] R. L. Hayes, J. K. Noel, P. C. Whitford, U. Mohanty, K. Y. Sanbonmatsu, J. N. Onuchic. Reduced model captures Mg^{2+}-RNA interaction free energy of riboswitches. *Biophys. J.* **106**, 1508, 2014.

[26] P. C. Whitford*, S. C. Blanchard, J. H. D. Cate, K. Y. Sanbonmatsu. Connecting the kinetics and energy landscape of tRNA translocation on the ribosome. *PLoS Comp. Biol.* **9**, e1003003, 2013.

[25] P. C. Whitford*, K. Y. Sanbonmatsu*. Simulating movement of tRNA motion through the ribosome during hybrid-state formation. *J. Chem. Phys.* **139**, 121919, 2013.

[24] J. Wang, R. J. Oliveira, X. Chu, P. C. Whitford, J. Chahine, W. Han, E. Wang, J. N. Onuchic, V. B. P. Leite. Topography of funneled landscapes determines the thermodynamics and kinetics of protein folding. *Proc. Nat. Acad. Sci. USA.* **109**, 15763-15768, 2012.

[23] R. L. Hayes, J. K. Noel, U. Mohanty, P. C. Whitford, S. P. Hennelly, J. N. Onuchic, K. Y. Sanbonmatsu. Magnesium fluctuations modulate RNA dynamics in the SAM-1 riboswitch. *J. Amer. Chem. Soc.* **134**, 12043-12053, 2012.

[22] M. A. Jamros, L. C. deOliveira, P. C. Whitford, J. N. Onuchic, J. A. Adams, and P. A. Jennings. Substrate-specific reorganization of the conformational ensemble of CSK implicates novel modes of kinast function. *PLoS Comp. Biol.* **8**, e1002695, 2012.

[21] J. K. Noel, P. C. Whitford and J. N. Onuchic. The shadow method: A generally-applicable contact definition for capturing the dynamics of biomolecular folding and function. *J. Phys. Chem.* **116**, 8692-8702, 2012.

[20] J. Singh, P. C. Whitford, N. Hayre, J. N. Onuchic and D. Cox. Massive conformation change in the prion protein: Using dual-basin structure-based models to find misfolding pathways. *Proteins: Struct. Func. Bioinfo.* **80**, 1299-1307, 2012.

[19] A. Ahmed, P. C. Whitford, K. Y. Sanbonmatsu and F. Tama. Consensus between flexible fitting computational methods to interpret cryo-EM data. *J. Struct. Biol.* **177**, 561-570, 2012.

[18] P. C. Whitford, A. Ahmed, Y. Yu, S. P. Hennelly, F. Tama, C. M. T. Spahn, J. N. Onuchic and K. Y. Sanbonmatsu. Excited states of ribosome translocation revealed through integrative molecular modeling. *Proc. Nat. Acad. Sci. USA.* **108**, 18943-18948, 2011.

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Last Updated: June 7, 2022