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# ROHIT V. PAPPU

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## PROFESSIONAL BACKGROUND

### *Positions*

**March 2015 – current:** Edwin H. Murty Professor of Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences

**January 2013 – current:** Co-Director, Center for High Performance Computing, Washington University in St. Louis

**September 2012 – current:** Director, Center for Biological Systems Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences

**January 2011 – current:** Professor, Department of Biomedical Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences

**March 2007 – current**: Member, Hope Center for Neurodegenerative Disorders, Washington University School of Medicine

**July 2007 – December 2010**: Associate Professor, Department of Biomedical Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences; Adjunct Associate Professor, Department of Biochemistry & Molecular Biophysics, Washington University School of Medicine

**February 2009 – August 2010:** Director, Center for Computational Biology, Washington University School of Medicine

**May 2002 – August 2010**: Member, Center for Computational Biology, Washington University School of Medicine

**September 2001 – June 2007**: Assistant Professor, Department of Biomedical Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences; Adjunct Assistant Professor, Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine

### *Education and training*

**Postdoctoral Scientist**, 1998-2001
Department of Biophysics and Biophysical Chemistry, Johns Hopkins University, School of Medicine, Baltimore, MD; Mentor: Professor George D. Rose

**Postdoctoral Scientist**, 1996-1998

Department of Biochemistry and Molecular Biophysics, Washington University in Saint Louis, School of Medicine, St. Louis, MO; Mentor: Professor Jay W. Ponder

**Ph.D.**, Biological Physics, 1992-1996
Department of Physics and Astronomy, Tufts University, Medford, MA
Advisor: Professor David L. Weaver (deceased)
Thesis: Algorithms for modeling folding pathways of proteins.

**M.S.**, Solid State Physics, 1990-1992
Department of Physics and Astronomy, Tufts University, Medford, MA

**B.Sc.**, Honors in Physics, Mathematics, and Electronics, 1986-1989
St. Joseph's College, Bangalore University, Bangalore, India

## RESEARCH PROGRAM

### *Summary of research focus*

My research is focused on three topics: the molecular basis of neurodegeneration in Huntington's disease (HD) and Alzheimer's disease (AD), the phase behavior of protein and RNA molecules driven by intrinsically disordered proteins (IDPs), and the control of cellular processes and decision making circuits by IDPs. Our discoveries are driven by a blend of multiscale computer simulations, development of novel computational approaches, adaptations of polymer physics theories, combinations of *in vitro* experiments, and collaborations that enable cellular level investigations.

**Neurodegeneration:** We have developed a quantitative mechanistic framework to describe polyglutamine-mediated aggregation. We have also uncovered how aggregation is modulated by the synergy between polyglutamine length and flanking sequence contexts. We are beginning to connect the process of polyglutamine aggregation to intracellular interactions that lead to neurodegeneration in HD and other polyglutamine expansion disorders. We are transferring ideas gleaned from the study of protein aggregation in HD to understand how Amyloid beta (Aβ) and Tau aggregation are modulated by endogeneous extracellular proteins (Aβ) and how conformational strains emerge for Tau aggregates.

**Intrinsically disordered proteins (IDPs):** These proteins are abundant in eukaryotic proteomes and are implicated in important cellular functions that underlie transcriptional regulation and signal transduction. IDPs fail to fold as autonomous units and yet they feature prominently in functions that control cellular processes with direct implications for cancers, developmental, and cardiovascular disorders. We have developed and used novel combinations of polymer physics theories, molecular simulations, and biophysical experiments to provide definitive descriptors relating for the relationships between information encoded in IDP sequences and their conformational properties. We are using *de novo* sequence design to modulate conformational properties of IDPs and quantify the impact of these changes on functions of specific IDPs and the distinct cellular processes they control.

**Phase transitions and intracellular compartmentalization**: We have considerable interest in the problem of phase transitions that are controlled or influenced by IDPs. These phase transitions include phase separation, sol-gel transitions, and convolution between the two. We are developing novel multiscale, multiresolution methods to understand the driving forces for, mechanisms of, and functions associated with membraneless organelles that form as the result of phase transitions.

### *Awards – Reverse Chronological Order*

Elected to the American Institute for Medical and Biological Engineering (AIMBE) College of Fellows, April 2016

Installed as the Edwin H. Murty Professor of Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences, March 2015

Elected fellow of the American Association for Advancement of Science (AAAS), November 2013

Basil O'Connor Starter Scholar Award, March of Dimes Research Foundation, 2004

Graduate Biophysics Fellowship, selected to attend Princeton-NEC workshop, June 1996

John F. Burlingame Graduate Research Fellowship, Tufts University, 1995 – 1996

National Merit Scholarship, Bangalore University, Bangalore, India, 1989

### *Honors – Reverse Chronological Order*

Member of the executive committee of the Human Dark Proteome Initiative

Invited to give the Telluride town talk entitled "Neurodegeneration from the ground up" as an accompaniment to the Telluride Science Research Conference Series, July 2015

Elected to chair the 2017 FASEB Summer Research Conference on Molecular Mechanisms and Physiological Consequences of Protein Aggregation

Guest Editor, Special Issue of Seminars on Cell and Developmental Biology, 2015

Member, Editorial Advisory Board, Biophysical Journal, December 2014 – July 2016

Member, Executive Committee, Protein Folding Consortium, Sponsored by the National Science Foundation, Research Coordination Network, September 2014 – current

Member, Editorial Board of Protein Engineering, Design and Selection, July 2014 – current

Elected Symposium Co-Chair for the 9th Annual Symposium of the Biophysical Society's Intrinsically Disordered Proteins Subgroup, February 2014

Faculty 1000 Member, Structural Biology: Theory & Simulation Section, April 2013 – current

BMC Biophysics, Editorial Board Member, 2012 – current

Chair, 2nd Gordon Research Conference on Intrinsically Disordered Proteins, 2012

One of Fifteen Scientists Invited by the National Science Foundation to Participate in a Workshop to Discuss the Future and Frontiers of Protein and RNA Biophysics, September 2011

Charter Member, National Institutes of Health Center for Scientific Review, Biophysics of Neural Systems Study Section, June 2008 – June 2012

Member, Protein Folding Consortium, Supported by the National Science Foundation, Research Coordination Network, May 2009 – current

Chair, by election, Intrinsically Disordered Proteins Subgroup, Biophysical Society, 2009

Regular Member, National Science Foundation, Molecular & Cellular Biosciences, Biophysics Panel, April 2008 – Current

### *Invited Talks at National and International Meetings – Reverse Chronological Order*

Invited Speaker, 3rd International Workshop on Protein Folding & Dynamics, National Centre for Biological Sciences, Bengaluru, India, November 2016

Invited Speaker, 2nd COST Symposium on Non-Globular Proteins in Molecular Pathophysiology, Belgrade, Serbia, September 2016

Invited Speaker, Physical Chemistry Division Symposium In Intrinsically Disordered Proteins at the 252nd National Meeting of the American Chemical Society, August 2016

Invited Speaker, 30th Anniversary Symposium of the Protein Society, July 2016

Invited Speaker, 3rd Workshop on the Physical Basis of Cellular Adaptation & Memory, Bellairs Research Institute, Barbados, April 2016

Invited Speaker, CHDI Htt Protein Lifecycle Workshop, New York City, March 2016

Invited Symposium Speaker, 60th Annual Meeting of the Biophysical Society, Los Angeles, CA March 2016

Invited Keynote Speaker, International Symposium on Chromatin Dynamics: Theoretical and Polymer Physics Approaches, Hiroshima, Japan, December 2015

Invited Speaker, Southeast and Southwest regional meeting of the American Chemical Society, Symposium on Intrinsically Disordered Proteins, Memphis, TN, November 2015

Invited Opening Plenary Speaker, 12th Annual New England Structure Symposium (NESS), Theme: Structure and Dynamics of Intrinsically Unfolded Proteins, sponsored by the University of Connecticut, Storrs, CT, October 2015

Invited Keynote Speaker, 29th Annual Gibbs Conference on Biothermodynamics, Touch of Nature Conference Center, Carbondale, IL October 2015

Invited Keynote Speaker at the Annual Symposium of the Cellular Dynamics and Macromolecular Complexes CREATE Graduate Training Program, University of Montreal, Canada, August 2015

Invited Speaker, CECAM Workshop on Computational Modeling of Intrinsically Disordered Proteins, Zurich, Switzerland August 2015

Invited Speaker, FASEB meeting on Molecular Mechanisms and Physiological Consequences of Protein Aggregation, June 2015

Invited Speaker, Proteins Gordon Research Conference, Holderness, New Hampshire, June 2015

Invited Speaker, Conference on Intracellular Phase Transitions: RNA, Protein, Lipids, and Beyond. Princeton University, April 2015

Invited Speaker, International Scientific Seminar, Chromosome Dynamics: Computational Models and Experimental Data, Sponsored by the Royal Society, Chicheley Hall, Buckinghamshire, UK, November 2014

Invited Speaker and Session Chair, Thematic Meeting, Disordered Motifs and Domains in Cell Control, Dublin Ireland – Sponsored by the Biophysical Society, October 2014

Invited Keynote Speaker, Intrinsically Disordered Proteins Gordon Research Conference, July 2014

Invited Keynote Speaker, 8th Annual Symposium of the Biophysical Society's Intrinsically Disordered Proteins Subgroup, February 2014

Invited Speaker, Gordon Research Conference on Protein Folding Dynamics, January 2014

Invited Speaker, 3rd USA-Mexico Workshop in Biological Chemistry: Protein Folding, Dynamics, and Function, November 2013

Invited Speaker, CECAM International Workshop on Intrinsically Disordered Proteins, ETH Zurich, September 2013

Invited Speaker, FASEB Summer Research Conference on Molecular Mechanisms and Physiological Consequences of Protein Aggregation, June 2013

Invited Speaker, 57th Annual Meeting of the Biophysical Society, February 2013

Invited Speaker, International Symposium on Protein Folding, National Centre for Biological Sciences, Bangalore, India, October 2012

Invited Speaker, Biopolymers Gordon Research Conference, June 2012

Invited Keynote Speaker, Annual Midwest Conference on Protein Folding, Assembly, and Molecular Motions, May 2011

Invited Speaker, Gordon Research Conference on Protein Folding Dynamics, January 2010

Invited Speaker, FASEB Summer Research Conference on Biophysics and Biology of Amyloids, June 2009

Invited Speaker and Session Chair, 53rd Annual Meeting of the Biophysical Society, March 2009

Invited Speaker, 22nd Annual Symposium of The Protein Society, July 2008

Invited Speaker, Biopolymers Gordon Research Conference, June 2008

Invited Speaker and Symposium Co-Chair, 2nd Annual Symposium of the Biophysical Society's Intrinsically Disordered Proteins Subgroup, February 2008

Invited Speaker, FASEB Amyloid Meeting, June 2006

Invited speaker, I2CAM Workshop on Protein Aggregation and Amyloid Formation in Systemic and Neurodegenerative Diseases, EPFL, Lausanne, Switzerland, July 2005

### *Awards & Honors to Members of the Lab – Reverse Chronological Order*

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, was one of the awardees for best posters presented at the fourth biennial Intrinsically Disordered Proteins Gordon Research Conference held in Les Diabrelets, Switzerland in June 2016.

Mr. Alex Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab was elected as co-chair of the 2018 Graduate Research Seminar that is to accompany the fifth biennial Intrinsically Disordered Proteins Gordon Research Conference.

Mr. Tyler Harmon, Physics Graduate Student in the Pappu Lab was named as one of the CBSE Graduate Student Scholar by the Center for Biological Systems Engineering at Washington University for the period between July 01, 2016 and June 30, 2017.

Mr. Alex Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab was named as the Kent and Bonnie Lattig CBSE Graduate Student Scholar by the Center for Biological Systems Engineering at Washington University for the period between July 01, 2016 and June 30, 2017.

Mr. Alex Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab selected to give an invited talk at the Gordon Research Seminar preceding the Gordon Research Conference on Intrinsically Disordered Proteins, Les Diabrelets, Switzerland, June 2016.

Mr. Alex Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab gave an invited platform session talk at the 60th Annual Meeting of the Biophysical Society, February 2016.

Mr. Tyler Harmon, Physics Graduate Student in the Pappu Lab gave an invited platform session talk at the 60th Annual Meeting of the Biophysical Society, February 2016.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, was named the first Kent and Bonnie Lattig CBSE Graduate Student Scholar by the Center for Biological Systems Engineering at Washington University in St. Louis for the period between July 2015 and June 2016.

Mr. Tyler S. Harmon, Physics Graduate Student in the Pappu Lab, was chosen to give the opening talk at the 2015 edition of the annual meeting of the NSF sponsored Protein Folding Consortium, Berkeley, May 2015.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, was reappointed as a CBSE Graduate Student Scholar by the Center for Biological Systems Engineering at Washington University in St. Louis for the period between July 2015 and June 2016.

Ms. Kiersten Ruff, Computational & Systems Biology Graduate Students in the Pappu Lab was chosen to speak at the Princeton Workshop on Intracellular Phase Transitions, April 2015.

Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab, Recipient of the SRAA Award for Best Poster, 59th Annual Meeting of the Biophysical Society, Award Sponsored by the Intrinsically Disordered Proteins Subgroup, February 2015.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, Selected to deliver a platform session talk at the 59th annual meeting of the Biophysical Society, Baltimore, MD, February 2015.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, was appointed as a CBSE Graduate Student Scholar by the Center for Biological Systems Engineering at Washington University in St. Louis for the period between July 2014 and June 2015.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, Selected to speak at the first Graduate Research Seminar preceding the 3rd Gordon Research Conference on Intrinsically Disordered Proteins, Stonehill College, MA, June 2014.

Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab, Recipient of the SRAA Award for Best Poster, 58th Annual Meeting of the Biophysical Society, Award Sponsored by the Intrinsically Disordered Proteins Subgroup, February 2014.

Dr. Anuradha Mittal, Postdoc in the Pappu Lab, Selected to give a platform session talk at the 58th Annual Meeting of the Biophysical Society, San Francisco, February 2014.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, Recipient of the SRAA Award for Best Poster, 58th Annual Meeting of the Biophysical Society, Award Sponsored by the Intrinsically Disordered Proteins Subgroup, February 2014.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, Received Honorable Mention from National Science Foundation in response to Graduate Student Fellowship, with Enhanced Access to Cyberinfrastructure

Resources, Including XSEDE Supercomputing Time to Support Research Toward Completion of Graduate Program, 2013.

Ms. Kiersten M. Ruff, Computational & Systems Biology Graduate Student in the Pappu Lab, Recipient of the SRAA Award for Best Poster, 57th Annual Meeting of the Biophysical Society, Award Sponsored by the Intrinsically Disordered Proteins Subgroup, 2013.

Dr. Scott L. Crick, Recipient of the National Institutes of Health, National Research Service Award for Postdoctoral Research following the completion of thesis work and a two-year postdoctoral stint in the Pappu Lab, 2013.

Mr. Nicholas Lyle, Computational & Systems Biology Graduate Student, Best Poster Award, Intrinsically Disordered Proteins, Gordon Research Conference, 2012.

Dr. Scott L. Crick, Postdoc in the Pappu Lab, Selected to deliver a Platform Session Talk at the 56th Annual Meeting of the Biophysical Society, San Diego, CA, 2012.

Dr. Rahul K. Das, Postdoc in the Pappu Lab, Recipient of the Molecular Kinetics Postdoctoral Speaking Award and Honorarium, 5th Annual Symposium of the Intrinsically Disordered Proteins Subgroup at the 55th Annual Meeting of the Biophysical Society, Baltimore, MD, 2011.

Mr. Albert H. Mao, MSTP and Computational & Molecular Biophysics Graduate Student in the Pappu Lab, Recipient of the SRAA Award for Best Poster, 55th Annual Meeting of the Biophysical Society, Baltimore, MD, Award Sponsored by the Intrinsically Disordered Proteins Subgroup, 2011.

Mr. Scott L. Crick, Biomedical Engineering Graduate Student in the Pappu Lab, Selected to deliver a Platform Symposium Talk at the 54th Annual Meeting of the Biophysical Society, San Francisco, CA, 2010.

Dr. Matthew A. Wyczalkowski, Former Biomedical Engineering Graduate Student, Recipient of the National Institutes of Health, National Research Service Award for Postdoctoral Research following the completion of thesis work in the Pappu Lab, 2010.

Dr. Alan A. Chen, Former Computational & Molecular Biophysics Graduate Student, Recipient of the National Institutes of Health, National Research Service Award for Postdoctoral Research following the completion of thesis work in the Pappu Lab, 2010.

Dr. Andreas Vitalis, Computational & Molecular Biophysics Graduate Student Empiris Award for Research in Brain Diseases, Award received for Ph.D. thesis work performed in the Pappu Lab, 2010.

### *Peer Reviewed Publications (reverse chronological order) Includes peer reviewed book chapters and articles in press*

1. T.S. Harmon, M.D. Crabtree, S.L. Shammas, A.E. Posey, J. Clarke, R.V. Pappu. (2016). GADIS: Algorithm for designing sequences to achieve target secondary structure profiles of intrinsically disordered proteins. *Protein Engineering, Design, and Selection*, In press.

2. C.W. Pak. M. Kosno, A.S. Holehouse, S. Padrick, A. Mittal, R. Ali, A. Yunus, D. R. Liu, **R.V. Pappu***, M.K. Rosen*. (2016). Sequence determinants of intracellular phase separation via complex coacervation of a model disordered protein. *Molecular Cell,* **63**: 72-85. *Co-corresponding authors.

3. M. Feric, N. Vaidya, T.S. Harmon, D. M. Mitrea, L. Zhu, T.M. Richardson, R.W. Kriwacki, **R.V. Pappu**, C.P. Brangwynne. (2016). Coexisting liquid phases underlie nucleolar sub-

compartments. *Cell*. **165:** 1-12.

4. R.K. Das, Y. Huang, A. Phillips, R.W. Kriwacki, **R.V. Pappu**. (2016). Cryptic sequence features within the disordered protein p27$^{\mathrm{Kip1}}$ regulate cell cycle signaling. *Proceedings of the National Academy of Sciences USA*. **113:** 5616-5621.
5. S. Banjade, Q. Wu, A. Mittal, W. Peeples, **R.V. Pappu**, M.K. Rosen. (2015). A Conserved Interdomain Linker Promotes Phase Separation of the Multivalent Adaptor Protein Nck. *Proceedings of the National Academy of Sciences USA.* **112**: E6426 – E6435.
6. K.M. Ruff, T.S. Harmon, **RV. Pappu**. (2015). CAMELOT: A machine learning optimized approach for coarse-grained simulations aggregation of block-copolymeric protein sequences. *Journal of Chemical Physics*. **143**: 243123.
7. C.P. Brangwynne, P.S. Tompa, **R.V. Pappu**. (2015). Polymer Physics of Intracellular Phase Transitions. *Nature Physics*. **11**: 899-904.
8. A.S. Holehouse, **R.V. Pappu**. Encoding phase transitions. (2015). *Nature Materials*. **14**: 1083-1084. Invited News & Views piece.
9. R.K. Das, K.M. Ruff, **R.V. Pappu**. (2015). Relating sequence encoded information to form and function of intrinsically disordered proteins. *Current Opinion in Structural Biology.* **31:** 102-112.
10. M.I. Diamond, S. Cai, A. Boudreau, C.J. Carey Jr., N. Lyle, **R.V. Pappu**, S.J. Swamidass, M. Bissell, H. Piwnica-Worms, J. Shao. (2015). Subcellular localization and Ser-137 phosphorylation regulate tumor-suppressive activity of profilin-1. *Journal of Biological Chemistry*. **290:** 9075-9086.
11. P.J. Buske, A. Mittal, **R.V. Pappu**, P.A. Levin (2015). An intrinsically disordered linker plays a critical role in bacterial cell division. *Seminars in Cell and Developmental Biology*. **37**: 3-10.
12. **R.V. Pappu** (2015). Cell signaling, division, and organization mediated by intrinsically disordered proteins. *Seminars in Cell and Developmental Biology.* **37**: 1-2.
13. A.S. Holehouse, K. Garai, N. Lyle, A. Vitalis, **R.V. Pappu**. Quantitative assessments of the distinct contributions of polypeptide backbones amides versus sidechain groups to chemical denaturation of proteins. (2015). *Journal of the American Chemical Society*. **137**: 2984-2995.
14. A. Mittal, R.K. Das, A. Vitalis, **R.V. Pappu**. (2015). The ABSINTH implicit solvation model and forcefield paradigm for use in simulations of intrinsically disordered proteins. In *Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods*. Edited by M. Fuxreiter. Chapter 6, 181-203. CRC Press, Boca Raton, FL.
15. A.G. Kozlov, E. Weiland, A. Mittal, V. Waldman, E. Antony, N. Fazio, **R.V. Pappu***, T.M. Lohman*. (2015). Intrinsically disordered C-terminal tails of *E. coli* single-stranded DNA binding protein regulate cooperative binding to single stranded DNA. (2014). *Journal of Molecular Biology*. **427:** 763-774. *Co-corresponding authors. **Selected and evaluated by Faculty of 1000.**
16. L. Ripaud, V. Chumakova, M. Antonin, A. Hastie, S. Pinkert, R. Koerner, K.M. Ruff, **R.V. Pappu,** D. Hornburg, M. Mann, F. U. Hartl, M. S. Hipp. (2014) Overexpression of Q-rich prion-like proteins suppresses polyQ cytotoxicity and alters the polyQ interactome. *Proceedings of the National Academy of Sciences USA*. **111**: 18219-18224.

17. K. M. Ruff, S.J. Khan, **R.V. Pappu.** (2014). A coarse-grained model for polyglutamine aggregation modulated by amphipathic flanking sequences. *Biophysical Journal*, **107**: 1226-1235. **Highlighted on the Biophysical Journal Home Page, September 02-15, 2014.**
18. **R.V. Pappu**. (2014). Frozen In Beta. *Biophysical Journal*. **107:** 795-797. Invited New & Notable Piece.
19. W. Xu, M.R. Edwards, D.M. Borek, A.R. Feagins, A. Mittal, J.B. Alinger, K.N. Berry, B.Yen, J. Hamilton, T.J. Brett, **R.V. Pappu**, D.W. Leung, C.F. Basler, G.K. Amarasinghe. (2014). Mechanism of cell-intrinsic innate immune antagonism by Ebola virus VP24. *Cell Host & Microbe*. **16:** 187-200. **Featured free article.**
20. A. Mittal, N. Lyle, T. S. Harmon, **R. V. Pappu**. (2014) Hamiltonian Switch Metropolis Monte Carlo Simulations for Improved Conformational Sampling of Intrinsically Disordered Regions Tethered to Ordered Domains of Proteins. *Journal of Chemical Theory and Computation*.**10:** 3550-3562.
21. A. Vitalis, **R.V. Pappu**. (2014). A Simple Molecular Mechanics Integrator in Mixed Rigid Body and Dihedral Angle Space. *Journal of Chemical Physics*. **141:** 034105(1-18).
22. A. T. Tubbs, Y. Dorsett, E. Chan, B. Helmink, B. Lee, P. Hung, R. George, A. L. Bredemeyer, A. Mittal, **R. V. Pappu**, D. Chowdhury, N. Mosammaparast, M. S. Krangel, B. P. Sleckman. (2014). KAP-1 Promotes Resection of Broken DNA Ends Not Protected by γ-H2AX and 53BP1 in G1-Phase Lymphocytes. *Molecular and Cellular Biology.* **34:** 2811-2821. PMID: 24842905.
23. R. van der Lee, M. Buljan, B. Lang, R. J. Weatheritt, G.W. Daughdrill, A. K. Dunker, M.Fuxreiter, J. Gough, J. Gsponer, D. T. Jones, P. M. Kim, R. W. Kriwacki, C. J. Oldfield, **R. V. Pappu**, P. Tompa, V. N. Uversky, P. E. Wright, M. M. Babu. (2014). Classification of intrinsically disordered regions and proteins. *Chemical Reviews*. **114**: 6959-6631. PMID: 24773235.
24. B. Luan, N. Lyle, **R.V. Pappu**, D.P. Raleigh. (2014). Denatured state ensembles with the same radius of gyration can form significant different long-range contacts. *Biochemistry*. **53:** 39-47. PMID: 24280003.
25. S.L. Crick, K.M. Ruff, K. Garai, C. Frieden, **R.V. Pappu**. Unmasking the roles of N- and C-terminal flanking sequences from exon 1 of huntingtin as modulators of polyglutamine aggregation. *Proceedings of the National Academy of Sciences USA*. **110:** 20075-20080. PMID: 2482292. **Article featured on Eureka Alert! http://www.eurekalert.org/pub_releases/2013-12/wuis-sao121113.php.**
26. R.K. Das, **R.V. Pappu**. (2013). Conformations of intrinsically disordered proteins are influenced by linear sequence distributions of oppositely charged residues. *Proceedings of the National Academy of Sciences USA*. **110:** 13392-13397. PMID: 23909099.
27. A.K. Dunker et al. (2013). What's in a name? Why these proteins are called intrinsically disordered? *Intrinsically Disordered Proteins*. **1**: e24157.
28. N. Lyle, R.K. Das, **R.V. Pappu**. (2013). A quantitative measure for protein disorder. *The Journal of Chemical Physics*. **139**: 121907. PMID: 24089719.
29. W. Meng, B. Luan, N. Lyle, **R.V. Pappu**, D.P. Raleigh. (2013). The Denatured State Ensemble Contains Significant Local and Long-range Structure Under Native Condition: Analysis of the N-terminal Domain of the Ribosomal Protein L9. *Biochemistry*, **52:** 2662-2671. PMID: 23480024.

30. W. Meng*, N. Lyle*, B. Luan, D.P. Raleigh, **R.V. Pappu**. (2013). Experiments and simulations show how long-range contacts can form in expanded unfolded proteins with negligible secondary structure. *Proceedings of the National Academy of Sciences USA*. **110:** 2123-2128. PMID: 23341588. *Co-first authors.
31. R.K. Das, A. Mittal, **R.V. Pappu**. (2013). How is functional specificity achieved through disordered regions of proteins? *BioEssays*, **35**: 17-22. PMID: 23138868.
32. A.H. Mao, N. Lyle, **R.V. Pappu**. (2013). Describing sequence-ensemble relationships for intrinsically disordered proteins. *Biochemical Journal*, **449**: 307-318. PMID: 23240611. (*Cover picture*)
33. M.M. Babu, R.W. Kriwacki, **R.V. Pappu**. (2012). Versatility from protein disorder. *Science*, **337**: 1460-1461. PMID: 22997313.
34. A.H. Mao, **R.V. Pappu**. (2012). Crystal lattice properties fully determine short-range interaction parameters for alkali and halide ions. *The Journal of Chemical Physics*. **137**: 064104(1-9). PMID: 22897252.
35. A. Radhakrishnan, A. Vitalis, A.H. Mao, A.T. Steffen, **R.V. Pappu**. (2012). Improved atomistic Monte Carlo simulations demonstrate that poly-L-proline adopts heterogeneous ensembles of conformations of semi-rigid segments interrupted by kinks. *Journal of Physical Chemistry B,* **116:** 6862-6871. PMID: 22329658.
36. R.K. Das, A.H. Mao, **R.V. Pappu**. (2012). Unmasking functional motifs within disordered regions of proteins. *Science Signaling*, **5**: pe17. PMID: 22510467.
37. R.K. Das, S.L. Crick, **R.V. Pappu**. (2012). N-terminal segments modulate the α-helical propensities of the intrinsically disordered basic regions of bZIP proteins. *Journal of Molecular Biology*, **416**: 287-299. PMID: 22226835.
38. S.L. Crick, **R.V. Pappu**. (2012). Thermodynamic and Kinetic Models for Aggregation of Intrinsically Disordered Proteins. *Book chapter in Peptide Folding, Misfolding, and Nonfolding.* Pg., 413-440. Ed. Reinhard Schweitzer-Stenner, Vladimir Uversky. John Wiley & Sons, Hoboken, NJ.
39. A. Vitalis, **R.V. Pappu**. (2011). Assessing the contribution of heterogeneous distributions of oligomers to aggregation mechanisms of polyglutamine peptides. *Biophysical Chemistry*, **159**: 14-23. PMID: 21530061.
40. R. Halfmann, S. Alberti, R. Krishnan, N. Lyle, C.W. O'Donnell, O.D. King, B. Berger, **R.V. Pappu**, S. Lindquist. (2011). Opposing effects of glutamine and asparagine govern prion formation by intrinsically disordered proteins. *Molecular Cell*, **43**: 72-84. PMID: 21726811.
41. A.H. Mao, **R.V. Pappu**. (2011). Exact recording of Metropolis-Hastings-class Monte Carlo simulations using one bit per sample. *Computer Physics Communications*. **182**: 1452-1454.
42. D.G. Thomas, **R.V. Pappu**, Baker, NA. (2011). NanoParticle ontology for cancer nanotechnology research. *Journal of Biomedical Informatics*. **44**: 59-74. PMID: 20211274.
43. M.A. Wyczalkowski, A. Vitalis, **R.V. Pappu**. (2010). New estimators for calculating solvation entropy and enthalpy and comparative assessments of their accuracy and precision. *Journal of Physical Chemistry B*, **114**: 8166-8180. PMID: 20503993.

44. A.H. Mao, S.L. Crick, A. Vitalis, C. Chicoine, **R.V. Pappu**. (2010). Net charge per residue modulates conformational ensembles of intrinsically disordered proteins. *Proceedings of the National Academy of Sciences USA*, **107**: 8183-8188. PMID: 20404210.
45. T.E. Williamson, A. Vitalis, S.L. Crick, **R.V. Pappu**. (2010). Modulation of polyglutamine conformations and dimer formation by the N-terminus of Huntingtin. *Journal of Molecular Biology*, **396**: 1295-1309. PMID: 20026071.
46. X. Hu, S.L. Crick, G. Bu, C. Frieden, **R.V. Pappu**, J-M. Lee. (2009). Amyloid seeds formed by cellular uptake, concentration, and aggregation of the amyloid-beta peptide. *Proceedings of the National Academy of Sciences USA*, **106**: 20324-20329. PMID: 19910533.
47. D.G. Thomas, **R.V. Pappu**, N.A. Baker. (2009). NPO: Ontology for Cancer Nanotechnology Research. *Nature Precedings.* EMBC 2009. http://dx.doi.org/10.1109/IEMBS.2009.5333941.
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***Submitted Manuscripts***

1. E.W. Martin, A.S. Holehouse, **R.V. Pappu**, T. Mittag. Sequence determinants of the conformational properties of an intrinsically disordered protein prior to and upon phosphorylation. *Journal of the American Chemical Society, under review.*

***Manuscripts in preparation***

1. A.E. Posey, K.M. Ruff, A.S. Holehouse, T.S. Harmon, M.I. Diamond, **R.V. Pappu**. Profilin binding suppresses huntingtin exon 1 aggregation and phase separation via polyphasic linkage.
2. T.S. Harmon, M.K. Rosen, **R.V. Pappu**. Linkers modulate phase transitions in multidomain signaling proteins.
3. A. Mittal, A.S. Holehouse, **R.V. Pappu**. Conformational properties of intrinsically disordered regions tethered to folded domains of proteins.
4. K. Sherry, R.K. Das, D. Barrick, **R.V. Pappu**. Control of transcriptional activity through *de novo* design of sequence-to-conformation relationships of the intrinsically disordered RAM region of the Notch intracellular domain.
5. K. Garai, X. Li, E.M. Powers, J. Buxbaum, **R.V. Pappu**. Transthyretin inhibits fibril formation and promotes the formation of insoluble amorphous aggregates through co-aggregation with Abeta oligomers.
6. K.M. Ruff, A.S. Holehouse, **R.V. Pappu**. Computational methods for multiscale simulations of intrinsically disordered proteins. *Invited review in preparation for Quarterly Reviews in Biophysics.*
7. A. S. Holehouse, R.K. Das, J. Ahad, M.O.G. Richardson, **R.V. Pappu**. CIDER: An online resource for classification of intrinsically disordered ensemble regions.
8. T.S. Harmon, A.E. Posey, **R.V. Pappu**. Charge patterned sequences form stable alpha helices through regulation of protonation states.
9. T.S. Harmon, A.S. Holehouse, K.M. Ruff, C.P. Brangwynne, **R.V. Pappu**. Physical concepts that govern the phase behavior of intrinsically disordered proteins. *Invited review in preparation for Biophysical Journal.*
10. A.S. Holehouse, **R.V. Pappu**. PIMMS: A novel lattice-based approach for modeling the sequence-specific phase behavior of intrinsically disordered proteins.

11. A.E. Posey, M. Cohan, S. Grigsby, A. Mittal, A.S. Holehouse, P. A. Levin, **R.V. Pappu**. Impact of the C-terminal intrinsically disordered tail of FtsZ on cell division in *B. subtilis*.
12. M. Crabtree, T.S. Harmon, R. Verma, J. Clarke, **R.V. Pappu**, S.L. Shammas. Mechanisms of coupled folding and binding modulated by sequences of fixed composition and rationally designed alterations to intrinsic helicities in intrinsically disordered proteins.
13. K. M. Ruff, **R.V. Pappu**. Synergistic modulation of polyglutamine conformations and associations by N- and C-terminal flanking sequences of huntingtin.
14. K.M. Ruff, **R.V. Pappu**. Evidence for nucleation independent sub-diffusive mechanisms for polyglutamine aggregation mediated by N-terminal flanking sequences.

***Grants – current, pending, and completed***

**CURRENT**

**National Institutes of Health, 1RO1GM108785**
**Title:** *Signal transduction by ERBB2 / ERBB3 oligomers*
**Funding period:** October 01, 2013 – September 30, 2017
**Principal Investigator:** Linda J. Pike
**Role in the project:** Co-Investigator

**National Institutes of Health, 1R01 NS089932-A1**
**Title**: *Mechanism of modulation of huntingtin exon 1 aggregation by profilin*
**Funding period:** April 01, 2016 – March 31, 2021
**Principal Investigators:** Marc I. Diamond, Ralf Langen, **Rohit Pappu (contact PI)**
**Role in the project:** Contact and Main PI in multi-PI grant

**National Institutes of Health (NINDS), 5R01NS056114-10-14**
**Title**: *Role of chain length and sequence contexts on polyglutamine oligomerization*
**Funding period:** July 01, 2016 – June 30, 2021
**Role in the project:** PI

**National Science Foundation, MCB-1614766**
**Title:** *Multiscale Modeling of Phase Transitions Driven by Multivalency and Disordered Proteins*
**Requested funding period:** August 01, 2016 – July 31, 2020
**Role in the project:** Principal Investigator
**Current status:** To be funded

**PENDING**

**COMPLETED**

**National Institutes of Health (NINDS), 5R01NS056114-05-09**
**Title:** *Role of chain length and sequence contexts on polyglutamine oligomerization*
**Funding period:** July 01, 2011 – June 30, 2016
**Role in the project:** PI

**National Science Foundation, MCB-0718924**
*Title: Phase behavior of intrinsically disordered proteins*
**Funding period:** September 01, 2011 – August 31, 2015
**Role in the project:** Principal Investigator

**National Institutes of Health, 1S10OD018091 Shared Instrumentation Grant**
**Title:** *GPU computing resource to enable innovation in imaging and network biology*
**Funding period:** April 01, 2014 – March 31, 2015
**Role in the project:** Co-PI with Fred Prior

**National Institutes of Health (NINDS), 5R01NS056114**
**Title:** *Atomistic studies of nucleation and oligomerization in polyglutamine aggregation*
**Funding period:** April 15, 2007 – June 30, 2012
**Role in the project:** PI

**National Science Foundation, MCB-0718924**
**Title:** *Conformational equilibria of intrinsically disordered proteins*
**Funding period:** September 01, 2007 – August 31, 2011
**Role in the project:** PI

**Hope Center for Neurological Disorders, Washington University School of Medicine**
Translational Neuroscience Pilot Project
**Title:** *Mechanism of Huntingtin Aggregation Regulated by Profilin*
**Funding period:** June 01, 2011 – May 31, 2013
**Role in the project:** Principal Investigator
**Co-Investigator:** Marc Diamond

**National Institutes of Health (NCI) U54 CA-119342**
**Title:** *An informatics resource for targeted nanoparticle therapeutics*
NCI Center grant to the Siteman Center for Cancer Nanotechnology Excellence (Center grant **PI:** Samuel Wickline)
**Funding period:** February 01, 2006 – January 31, 2011
**Role in the project:** Project Principal Investigator
**Project Co-Investigators**: David Sept, Nathan Baker

**Pfizer Inc., St. Louis, MO**
**Title:** *Modeling the aggregation of therapeutic monoclonal antibodies*
**Funding period:** October 31, 2009 – September 30, 2010
**Role in the project:** Project Principal Investigator

**National Institutes of Health (NCI) Integrated Cancer Research Workspace 94358NBS23**
*Subcontract for with Booz Allen Hamilton for Nanotechnology working group*
**Funding period:** April 01, 2008 – February 14, 2009
**Role in the project:** Principal Investigator

**National Science Foundation, MCB-0416766**
**Title:** *Studying the origin of conformational preferences in unfolded proteins*
**Funding period:** September 01, 2004 – August 31, 2007
**Role in the project:** Principal Investigator

**Hope Center for Neurological Disorders, Washington University School of Medicine**
Translational Neuroscience Pilot Project
**Title:** *Investigation of structural changes induced in amyloid Aβ fibrils by polyphenols*
**Funding period:** January 01, 2007 – December 31, 2007
Role in the project: Co-Investigator (PI: Jin-Moo Lee)

**Fidelity Foundation**
**Title:** *Studies on the process of aggregation in Huntington's disease*
**Funding period:** January 01, 2006 – December 31, 2006
Role in the project: Principal Investigator

**March of Dimes Birth Defects Foundation, Basil O'Connor Starter Scholar Award**
**Title:** *Factors that determine amyloid formation in polyglutamine disorders*
**Funding period:** February 01, 2004 – June 30, 2006
Role in the project: Principal Investigator

**National Institutes of Health, NIA P50 AG05681-20**
Pilot grant from Alzheimer's Disease Research Center, Washington University
**Title:** *Toward a molecular understanding of polyglutamine disorders*
**Funding period:** May 01, 2003 – April 30, 2004
**Role in the project:** Principal Investigator

### *Software*

1. **CAMPARI**: A simulation engine that integrates several sampling methodologies including molecular dynamics, rigid body dynamics, Langevin dynamics, novel torsional molecular dynamics, and an extensive code base for Monte Carlo sampling of biological macromolecules (mainly proteins, but also supports nucleic acids). The package was developed mainly by Andreas Vitalis, building on a skeleton that was developed by Pappu in the early days of the lab's existence. CAMPARI can be used for efficient calculation of free energies of solvation, neat liquids, complex fluids, and peptides in explicit solvent. However, the main advantage is its support of implicit solvent paradigms for use in Monte Carlo simulations. It is this aspect that makes CAMPARI unique. Significant work in the Pappu lab has shown that Monte Carlo simulations are extremely useful for efficient sampling of conformational space in conjunction with implicit solvation models such as ABSINTH, which was also developed by Andreas Vitalis in the Pappu Lab. This model may be viewed as an efficient interpolation between the EEF1 and generalized Born (GB) paradigms. CAMPARI will also integrate support for the major variants of the GB framework to facilitate comparative calculations between different implicit solvation paradigms. The CAMPARI engine, first built around the ABSINTH model, was designed for answering questions regarding conformational and binding equilibria of intrinsically disordered polypeptides. However, it has wider usage and has gained acceptance as a *bona fide* engine in the biomolecular simulation community. CAMPARI is available for free download from http://campari.sourceforge.net.
2. **CIDER – Classification of Intrinsically Disordered Ensemble Regions:** CIDER is a webserver being developed by the Pappu Lab for calculating parameters relating to disordered protein sequences. Specifically, this will calculate various parameters that help translate primary sequence information into a better understanding of the conformational properties of disordered proteins. The server provides a ready-made annotation on the Mao-Das-Pappu diagram-of-states for IDPs. In addition, predictions from CIDER yield insights regarding emergent properties of IDPs such as the conversion of polyampholytic IDPs to polyelectrolytes and vice versa as the result of phosphorylation. Alex S. Holehouse, a graduate student in the Pappu lab, is developing CIDER.
3. **NPO – a nanoparticle ontology**: Data generated from cancer nanotechnology research are so diverse and large in volume that it is difficult to share and efficiently use them without informatics tools. In particular, ontologies that provide a unifying knowledge framework for annotating the data are required to facilitate the semantic integration, knowledge-based searching, unambiguous interpretation, mining and inferencing of the data using informatics methods. We developed a NanoParticle Ontology (NPO) within the framework of the Basic Formal Ontology (BFO), and implemented in the Ontology Web Language (OWL) using well-defined ontology design principles. The NPO is

accessible online at http://www.nano-ontology.org/. Dr. Dennis Thomas developed this effort, sponsored by the National Cancer Institute. He was a postdoctoral scientist in my group. He is now at the Pacific Northwest National Laboratory and also works in close collaboration with Dr. Nathan Baker.

## RESEARCH MENTORING

### *Current Doctoral and Undergraduate Students (alphabetical order)*

1. **Megan C. Cohan**, Doctoral Student, Department of Biomedical Engineering. Projected graduation date, May 2020.
2. **Tyler S. Harmon**, Doctoral Student, Department of Physics. Projected graduation date, January 2017.
3. **Alex S. Holehouse**, Doctoral Student, Division of Biology & Biomedical Sciences, Computational & Molecular Biophysics Program. Projected graduation date, May 2017.
4. **Jared Lalmansingh**, Doctoral Student, Department of Physics. Projected graduation date, May 2020
5. **Kiersten M. Ruff**, Doctoral Student, Division of Biology & Biomedical Sciences, Computational & Systems Biology Program. Projected graduation date, December 2016.

### *Current Postdoctoral and other Scientists (alphabetical order)*

1. **Ammon Posey,** Research Scientist

### *Lab alumni – reverse chronological order*

1. **Rajni Verma**, Postdoctoral Scientist, October 2015 – May 2016.
2. **Rahul Das**, Postdoctoral Scientist. Currently, a senior research fellow at The Rothberg Institute and Yale University.
3. **Anuradha Mittal**, Postdoctoral Scientist. Currently, a senior Bioinformatics Scientist at Affymetrix, San Francisco, CA.
4. **Mary O.G. Richardson**, Undergraduate Student, Class of 2017, Junior majoring in Biomedical Engineering & Bioinformatics.
5. **Laruen M. Bedell**, Undergraduate Student, Department of Biomedical Engineering. Currently, MS student in Mechanical Engineering & Materials Science at Washington University.
6. **Kanchan Garai**, Research Assistant Professor and Research Scholar, Center for Biological Systems Engineering. Currently, Assistant Professor at the TIFR Centre for Interdisciplinary Studies, Hyderabad, India.
7. **James Ahad**, Undergraduate student, Biomedical Engineering. Currently, an MSTP student at Case Western University School of Medicine.
8. **Scott L. Crick**, Doctoral Student, Biomedical Engineering. Received Ph.D. in August 2011. Completed a two-year Postdoc in the lab in July 2013. Currently working as a Licensing Associate in the Office of Technology Management at Washington University in St. Louis.

9. **Siddique J. Khan**, Postdoc, April 2012 – May 2013.
10. **Nicholas Lyle**, Doctoral Student, Computational & Systems Biology Program, Division of Biology & Biomedical Sciences. Received Ph.D. in May 2013. Currently, Senior Scientific Analyst at Partek Inc., Chesterfield, MO.
11. **Tony Wang**, Summer undergraduate researcher, Summer 2012.
12. **Marta Wells**, Summer undergraduate research, Summer 2011 and 2012. Currently a graduate student in Computational Biology at Carnegie-Mellon University.
13. **Albert H. Mao**, M.D.-Ph.D. student, Computational & Molecular Biophysics Program, Division of Biology & Biomedical Sciences. Received Ph.D. in August 2012. Currently doing his residency in anesthesiology at Harvard Medical School, Beth Israel Hospital.
14. **Jordan Nick**, Summer HHMI undergraduate fellow, Summer 2011.
15. **Kelly Culhane**, SURF student, Summer 2011. Currently, a Ph.D. student in Biochemistry & Biophysics at Yale University.
16. **Aditya Radhakrishnan**, Master's student (BS/MS), Summer 2010 – Summer 2011. Currently Ph.D. student in Computational & Molecular Biophysics at Johns Hopkins University.
17. **Nil Gural,** Undergraduate researcher, Spring 2011. Currently Ph.D. student in the Harvard-MIT Health Sciences Program.
18. **Adam T. Steffen**, Scientific programmer, Summer 2007 – December 2010. Currently a software engineer at Partek Inc., Chesterfield, MO.
19. **Alexander French**, Undergraduate researcher, Summer 2010. Currently graduate student in Biochemistry & Biophysics at the University of Chicago.
20. **Anil Kumar**, Postdoctoral scientist, December 2009 – August 2010. Currently a postdoc at the University of Toronto in synthetic organic chemistry.
21. **Caitlin L. Chicoine**, Undergraduate researcher, Summer of 2009, Graduated from Washington University, School of Engineering & Applied Sciences Valedictorian.
22. **Matthew A. Wyczalkowski**, Biomedical Engineering. Received his Ph.D. in December 2009. Currently a senior postdoctoral scientist at The Genome Institute, Washington University School of Medicine.
23. **Tim E. Williamson**, Molecular Biophysics Program, Division of Biology & Biomedical Sciences and Staff Scientist. Received MS in May 2009. Currently working as a technical officer at Monsanto Inc., St. Louis, MO.
24. **Andreas Vitalis**, Doctoral Student, Molecular Biophysics Program, Division of Biology & Biomedical Sciences. Received his Ph.D. in June 2009. Currently an independent research scientist completing his research habilitation in the Department of Biochemistry at the University of Zurich.
25. **Alan A. Chen**, Doctoral Student, Molecular Biophysics Program, Division of Biology & Biomedical Sciences. Received his Ph.D. in May 2009. Currently assistant professor of chemistry the University of Albany, RNA Institute.
26. **Jose Pulido**, Undergraduate Trainee, May 2008 – October 2008.
27. **Xiaoling Wang**, Research scientist, September 2004 – February 2008. Currently a staff scientist at Pfizer Inc. in St. Louis, MO.

28. **Hoang T. Tran**, Doctoral student, Biomedical Engineering. Received Ph.D. in December 2007. Currently a staff scientist in the drug discovery at the M.D. Anderson Cancer Center in Houston, TX.
29. **Alexander N. Drozdov**, Postdoctoral Scientist, September 2002 – April 2004. Currently at Mentor Graphics, San Jose, CA; Senior scientist in the photolithography research group.
30. **Magdalena Fus**, Undergraduate Trainee, September 2004 – May 2005.
31. **Tirath Patel**, Undergraduate Trainee, September 2004 – May 2005.

***Other Invited talks: Fall 2001 – present (reverse chronological order)***

1. MRC Laboratory of Molecular Biology, Cambridge, UK, June 2016
2. Johns Hopkins University, Department of Materials Science, April 2016
3. Hiroshima University, December 2015
4. Duke University, NSF-MRSEC, April 2015
5. University of British Columbia, Center for High-Throughput Biology, April 2015
6. Washington University in St. Louis, Biophysical Evening, January 2015
7. University of Texas Southwestern Medical Center, Department of Biophysics, December 2014
8. University of Cambridge, Department of Chemistry, November 2014
9. MRC Laboratory of Molecular Biology, Cambridge, UK, November 2014
10. Stony Brook University, Laufer Center for Quantitative Biology, November 2014
11. Kansas State University, Department of Biochemistry, April 2014
12. Ohio State University, Department of Biochemistry, Biophysics Program, April 2014
13. University of Montana, Department of Chemistry & Biochemistry, February 2014
14. Johns Hopkins University, Department of Biophysics, December 2013
15. University of Wisconsin-Madison, Department of Chemical & Biochemical Engineering, December 2013
16. University of Zurich, Department of Biochemistry, September 2013
17. The Scripps Research Institute, Department of Molecular & Experimental Medicine, July 2013
18. University of Texas Southwestern Medical Center, University Colloquium, July 2013
19. University of Texas Southwestern Medical Center, Green Center for Systems Biology, Special Seminar, July 2013
20. Symposium on Physics and Biology of Strongly Fluctuating Proteins, University of Maryland, May 2013
21. American Chemical Society Meeting, New Orleans, April 2013
22. University of Chicago, Institute for Biophysical Dynamics, April 2013
23. March Meeting of the American Physical Society, Baltimore, March 2013
24. CUNY City College of New York, Structural Biology Colloquium, March 2013
25. 57th Annual Meeting of the Biophysical Society, Philadelphia, Protein Electrostatics Symposium
26. University of Minnesota, Department of Biomedical Engineering, December 2012
27. Protein Folding Consortium, PIs meeting, Chicago, November 2012

28. International Symposium on Protein Folding, National Centre for Biological Sciences, Bangalore, India, October 2012
29. Protein Folding Consortium, SUNY Stony Brook, NY, June 2012
30. Biopolymers Gordon Research Conference, Newport, RI, June 2012
31. Hope Center for Neurological Disorders, Washington University, May 2012
32. Arizona State University, Center for Biological Physics, Tempe, AZ, April 2012
33. University of South Florida, Department of Physics, Tampa, FL, March 2012
34. St. Jude Children's Research Hospital, Memphis, TN, January 2012
35. CCP 2011 – Conference on Computational Physics, Knoxville, TN, November 2011
36. National Science Foundation Workshop on Future of RNA and Protein Folding, Arlington, VA, September 2011
37. University of Leeds, UK, July 2011
38. MRC Laboratory of Molecular Biology, Cambridge, UK, July 2011
39. Annual Meeting of the Protein Folding Consortium, UC Berkeley, June 2011
40. University of Texas Southwestern Medical School, May 2011
41. The Scripps Research Institute, Molecular & Experimental Medicine, May 2011
42. Washington University School of Medicine, Computational & Molecular Biophysics Program, Biophysical Evening Series, May 2011
43. Midwest Conference on Protein Folding, Assembly, and Molecular Motions, May 2011
44. 55th Annual Meeting of the Biophysical Society, Baltimore, MD, March 2011
45. Department of Biochemistry, Cornell Weill Medical College, December 2010
46. ACS Midwest Regional Meeting Symposium on Protein Folding, October, 2010
47. Intrinsically disordered proteins, Keynote Session Chair, Gordon Research Conference, North Carolina, July 2010.
48. Protein folding pathways workshop, Arizona State University, May 2010.
49. University of Pittsburgh School of Medicine, March 2010.
50. Yale University, Biophysics program, January 2010.
51. Protein folding and dynamics, Gordon Research Conference, January 2010.
52. The Scripps Research Institute, Molecular & Experimental Medicine, November 2009.
53. 23rd Annual Gibbs conference on Biothermodynamics, Carbondale, IL, October 2009.
54. Tata Institute of Fundamental Research, Mumbai, India, August 2009.
55. Argonne National Laboratory, Biology Division, August 2009.
56. Northwestern University, Biochemistry, Molecular Biology & Cell Biology, July 2009.
57. Telluride Scientific Research Conference, Workshop on RNA dynamics, July 2009.
58. FASEB Amyloid meeting, Snowmass, CO, June-July 2009.
59. University of California Berkeley, Department of Bioengineering, April 2009.
60. MIT-Whitehead Institute, Department of Biology, March 2009.
61. Annual Meeting of the Biophysical Society, Invited Workshop, Boston, MA, March 2009.
62. Department of Chemistry & Biochemistry, University of Massachusetts, Amherst, MA, February 2009
63. Rice University, Department of Chemistry, November 2009.
64. Rensselaer Polytechnic Institute, Biocomputation seminar series, October 2008.
65. 22nd Annual Symposium of the Protein Society, July 2008, San Diego, CA
66. Protein Electrostatics Workshop, Telluride, CO, July 2008
67. Biopolymers Gordon Research Conference, Newport, RI, June 2008.

68. University of Texas Austin, Department of Biomedical Engineering, April 2008.
69. University of Oregon, Department of Chemistry, April 2008.
70. Intrinsically Disordered Proteins subgroup meeting, Annual meeting of the Biophysical Society, Long Beach, CA, February 2008
71. The Scripps Research Institute, Department of Chemistry, La Jolla, CA, September 2007.
72. Gordon Research Conference: Proteins, June 2007, Holderness, New Hampshire.
73. Washington University in St. Louis, Biophysical Evening Series, December 2007.
74. University of California in Santa Barbara, Department of Chemistry, April 2007.
75. University of Delaware, Department of Chemistry and Biochemistry, April 2007.
76. Indiana University, Computational Biology and Bioinformatics, September 2006.
77. National Cancer Institute, Frederick, August 2006.
78. FASEB Amyloid Meeting, Snowmass, Colorado, June 2006.
79. DIMACS Workshop on Computational / Experimental Approaches to Protein Defects in Human Disease, Rutgers University, April 2006.
80. University of North Carolina, Chapel Hill, Department of Chemistry, April 2006.
81. Duke University, Department of Biochemistry, April 2006.
82. UTMB, Galveston, TX, Sealy Center for Structural Biology, April 2006.
83. Johns Hopkins University, Department of Chemistry, March 2006.
84. Stanford University, Department of Chemistry, March 2006.
85. I2CAM Exploratory Workshop on Protein Aggregation and Amyloid Formation in Systemic and Neurodegenerative Diseases: Physical, Molecular, and Biological Approaches, EPFL, Lausanne, Switzerland, July 2005.
86. 18th Annual Gibbs Conference on Biothermodynamics, Carbondale IL, October 2004.
87. University of Iowa, Department of Chemistry, Iowa City, May 2004.
88. Washington University, Alzheimer's disease Research Center, April 2004.
89. Washington University, Department of Genetics, October 2002.
90. Washington University, Alzheimer's disease Research Center, December 2002.
91. Washington University, Biophysical Evening Seminar Series, December 2001.

## TEACHING

1. *Bioengineering Thermodynamics*, BME 320B, Fall 2010 onward. Audience: Biomedical Engineering juniors.
2. *Applied Mathematics for Biomedical Sciences*, Fall 2013. Audience: Graduate students in Biomedical Engineering & quantitative programs in the Division of Biology & Biomedical Sciences.
3. *Chemical Thermodynamics*, ChemE 320 / BME 320,Fall 2008 and 2009. Audience: Chemical Engineering sophomores and Biomedical Engineering juniors.
4. *Biomedical Engineering Design*, BME 401, Fall 2007. Co-course master for the capstone senior design course. Audience: Biomedical Engineering seniors, and graduate students in BME and Molecular Biophysics.
5. *Principles of Protein Structure, BME 461*, Every Fall starting Fall 2003. Audience: Seniors and graduate students in Biomedical Engineering.

6. *Introduction to Biomolecular Statistical Thermodynamics, BME 531*, Graduate Level, Every Spring, starting Spring 2002. Audience: Graduate students in Biomedical Engineering, Chemical Engineering, and Molecular Biophysics. Last time course was taught: Spring 2007.
7. *Modeling Biomolecular Systems, Part II, BME 540*, Fall 2004. Audience: Graduate students in Biomedical Engineering, Chemical Engineering, Molecular Biophysics, and Computational Biology.
8. *Quantitative physiology, part II, BME 301B,* **Four Lectures** on *Applications of control theory in modeling physiological systems*, Spring 2003 – Spring 2005. Audience: Juniors majoring in Biomedical Engineering.
9. *Quantitative physiology, part II, BME 301B,* **Two Lectures** on the *Quantitative aspects of Antigen-Antibody Interactions and their role in control and regulation of immune response*, Spring 2006. Audience: Juniors majoring in Biomedical Engineering.

## LEADERSHIP EXPERIENCE

### *Leadership Within Washington University*

### Center for Biological Systems Engineering

I am the founding Director of the Center for Biological Systems Engineering (CBSE). This center is the home of network biology at Washington University and has incorporated researchers from the School of Engineering & Applied Science (SEAS) and the School of Medicine. These researchers deploy multiscale, systems-based approaches to model, predict and design functions of biological systems that result from the integration of signals and responses of biomolecular and cellular networks.

I led a cluster search to recruit suitable investigators to populate the CBSE. The search was successful in recruiting three new investigators, two by way primary appointments in Biomedical Engineering (BME), and one with primary appointment in Pathology & Immunology (P&I). Additionally, I recruited out to four kindred scientists from BME and P&I with expertise in multiscale approaches to challenging problems in biomedical science. Within a short period, I assembled a talented group of eight investigators, six of whom are assistant professors.

Research interests within the center span a range of topics including modeling protein self-assembly and homeostasis networks, reverse engineering networks controlled by post-translational modifications, utilizing and adapting novel sequencing methods to interrogate the organization of small RNA networks, chemical informatics geared toward prospecting for and repurposing novel small molecules, de novo design of protein interaction networks, and developing advanced imaging modalities for non-invasive interrogations of biological tissues.

### Center for High Performance Computing

I am currently the co-director, with Dr. Fred Prior, of the Center for High Performance Computing (CHPC) at Washington University. My close involvement with the CHPC has contributed to a fundamental improvement of the computational environment at Washington University, which was essentially non-existent a few years ago. This effort has required several delicate interactions and management of important issues, and I have learned to become proficient in cultivating inter-personal relationships that enable rather than compromise the success of projects.

**Department of Biomedical Engineering**

I have contributed mainly as a model citizen to the curricular and research programs within the BME department. In addition to participating on key departmental committees, I took the lead on two specific curricular matters. I took over the teaching of Thermodynamics for our BME undergraduates and redesigned this course to emphasize the importance of thermodynamics concepts across the molecular, cellular, and physiological scales. This initiative helped improve the synergy between thermodynamics and the two quantitative physiology courses that are taught in the department. I added a focused problem-solving module to this course. I proposed the idea of developing a new laboratory module to go along with this course, and this has come to fruition following the recruitment of a suitably qualified instructor to handle these duties. My efforts in Bioengineering Thermodynamics help illustrate my ability to craft a vision and see the vision through to fruition through earnest effort and refinement of the vision by incorporating critical feedback.

I have brought a similar approach to bear on the topic of developing a new applied mathematics course for biomedical sciences. I am currently teaching this course that I developed from scratch. It is being designed to provide a direct conduit from concept to application of mathematics in biology and biomedical sciences. It is the only course of its kind at Washington University and this has arisen entirely through my initiative.

From a research standpoint, I have been actively involved in faculty recruitment within BME, have chaired and been a member of search committees, and I was the primary author of the white paper that was crafted roughly two years ago for the future research mission of the BME department. In crafting this white paper, I worked closely with a key senior colleague in the department, and actively solicited and incorporated the inputs from all of my BME colleagues, thus showcasing my ability to be both visionary and collaborative.

## SERVICE

### *Professional activities*

1. Reviewer of manuscripts for the *Biochemical Journal*, *Biochemistry*, *Biomacromolecules, Biophysical Journal, Biophysical Chemistry, Journal of Chemical Physics, Journal of Molecular Biology, Journal of Physical Chemistry B, Structure, Journal of the American Chemical Society, Journal of Chemical Theory and Computation*, *Journal of Computational Chemistry, Nature, Proceedings of the National Academy of Sciences USA, PLoS: Computational Biology, PLoS One, Science Signaling, Structure.*
2. Panelist for review of National Science Foundation SBIR grants, Bioinformatics.
3. Panelist and reviewer of grants for National Science Foundation, Molecular & Cellular Biophysics.
4. Ad hoc reviewer for National Science Foundation, Biotechnology.
5. Grant Reviewer for Alzheimer's Disease Research Center, Washington University
6. Grant Reviewer for HighQ Foundation.
7. Co-author and contributor to Statement of Significance Petition to form a new Intrinsically Disordered Protein subgroup within the Biophysical Society.
8. Primary organizer of 1st International ICAM workshop on Multiscale Interactions and Dynamics in Complex Biological Systems, Washington University in Saint Louis, May 27-29, 2006.

9. Co-organizer for 20th Annual Gibbs Meeting on Biothermodynamics, October 7-10, 2006, Carbondale, IL.