

**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 interests**

My research is focused on four topics: the molecular basis of neurodegeneration in Huntington's disease (HD) and related disorders, phase transitions that lead to protein and RNA condensates driven by multivalent molecules, the biophysics of intrinsically disordered proteins, and design of responsive, protein-based biomaterials. Our work is driven by a blend of novel multiscale computer simulations, adaptations and developments of polymer physics and statistical physics theories, new ideas regarding the physics of living systems, *in vitro* and in cell experiments, and collaborations that enable molecular and cellular level investigations.

**Intrinsically disordered proteins (IDPs):** We have developed and used novel combinations of polymer physics theories, molecular simulations, and biophysical experiments to provide definitive descriptors 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.

**Neurodegeneration:** We work on connecting the driving forces for and the mechanisms of polyglutamine aggregation and phase separation to intracellular interactions that lead to neurodegeneration in HD and other polyglutamine expansion disorders. An emerging focus is on the modulation of aggregation and phase behavior by endogeneous networks of protein-protein interactions.

**Phase transitions in cell biology:** We have considerable interest in the problem of phase transitions that are controlled or influenced by multivalent proteins and RNA molecules. These phase transitions include phase separation, sol-gel transitions, the formation of liquid crystals, and the design of novel, stimulus responsive biomaterials. We are developing multiscale, multiresolution methods to understand the driving forces for, mechanisms of, and functions associated with membraneless organelles, also known as biomolecular condensates, that form as the result of phase transitions. This problem has direct relevance to spatiotemporal organization and information transduction within cells.

**Molecular and Cellular Engineering:** We are building on our work pertaining to phase transitions and IDPs to develop, prototype, and deploy computational methods to predict phase behavior from amino acid sequence and advance the design of responsive peptide and protein-based biomaterials.

***Awards – Reverse Chronological Order***

Dean's Award for Outstanding Contributions In Service of the Mission of the School of Engineering & Applied Sciences, Washington University in St. Louis, April 2017.

Syracuse Biomaterials Institute, Invited Keynote Distinguished Speaker, Syracuse University, April 2017.

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

Invited Keynote Speaker, 29<sup>th</sup> 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.

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

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

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

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***

Guest Editor, Current Opinion in Structural Biology, 2017

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 – current

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 9<sup>th</sup> Annual Symposium of the Biophysical Society's Intrinsically Disordered Proteins Subgroup, February 2014

Faculty 1000 Member, Structural Biology: Theory & Simulation Section, April 2013 – August 2016

BMC Biophysics, Editorial Board Member, 2012 – current

Chair, 2<sup>nd</sup> 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

***Notable Invited Talks at National and International Conferences***

Invited Speaker, Telluride Science Research Conference on Intrinsically Disordered Proteins and Membraneless Organelles, Telluride, CO, July 2017

Invited Speaker, Proteins Gordon Research Conference, Holderness, New Hampshire, June 2017

Invited Speaker, Inaugural symposium of the St. Jude Research Collaborative on membraneless organelles, The Biology of Liquid Organelles, St. Jude Children's Research Hospital, May 2017

Invited Speaker, New Frontier in Cellular Structure and Function, Genetics, Genomics and Systems Biology Symposium Sponsored by the University of Chicago, May 2017

Invited Speaker, VIB Conference Series, Phase Transitions in Biology and Disease, Leuven, Belgium, May 2017

Invited Speaker, Symposium on Coacervation: Physics, Chemistry, and Biology. Part of the 253<sup>rd</sup> National Meeting of the American Chemical Society, San Francisco, April 2017

Invited Speaker, 3<sup>rd</sup> International Workshop on Protein Folding & Dynamics, National Centre for Biological Sciences, Bangalore, India, November 2016

Invited Speaker, 2<sup>nd</sup> 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 252<sup>nd</sup> National Meeting of the American Chemical Society, August 2016

Invited Speaker, 30<sup>th</sup> Anniversary Symposium of the Protein Society, July 2016

Invited Speaker, 3<sup>rd</sup> 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, 60<sup>th</sup> 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, 12<sup>th</sup> 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 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 Speaker, Gordon Research Conference on Protein Folding Dynamics, January 2014
- Invited Speaker, 3<sup>rd</sup> 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, 57<sup>th</sup> 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, 53<sup>rd</sup> Annual Meeting of the Biophysical Society, March 2009
- Invited Speaker, 22<sup>nd</sup> Annual Symposium of The Protein Society, July 2008
- Invited Speaker, Biopolymers Gordon Research Conference, June 2008
- Invited Speaker and Symposium Co-Chair, 2<sup>nd</sup> 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**

- Dr. Kiersten M. Ruff, postdoctoral fellow in the Pappu Lab, was chosen to give a short talk at the 2017 FASEB Science Research Conference on Protein Aggregation in Health and Disease in Steam Boat Springs, CO, June 2017.
- Ms. Megan C. Cohan, Biomedical Engineering Graduate Student in the Pappu Lab, was chosen to give a student talk at the annual meeting of the NSF sponsored Protein Folding Consortium in Berkeley, CA, June 2017.
- Ms. Megan C. Cohan, Biomedical Engineering Graduate Student in the Pappu Lab, received a travel award to attend the 2017 annual meeting of the Biomedical Engineering Society to be held in Phoenix, AZ, October 2017.
- Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab gave a talk at the weeklong workshop on the Physics of Cellular Adaptation held at the Bellairs Institute in Barbados, April 2017.
- Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab, Recipient of the Spencer T. and Ann W. Olin for superior accomplishments in biomedical research doctoral students at Washington University, February 2017.
- Mr. Tyler S. Harmon, Physics Graduate Student in the Pappu Lab Recipient of the SRAA Award for Best Poster, 61<sup>st</sup> Annual Meeting of the Biophysical Society, Award Sponsored by the Intrinsically Disordered Proteins Subgroup, February 2017.
- Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab gave an invited platform session talk and chaired this session at the 61<sup>st</sup> Annual Meeting of the Biophysical Society, February 2017.
- Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab, received a student speaker award at the 23<sup>rd</sup> Annual retreat of the DBBS Computational & Molecular Biophysics Graduate Program for his talk entitled *Phase separation of intrinsically disordered proteins yields low-density “empty” liquids*.
- Ms. Megan C. Cohan, Biomedical Engineering Graduate Student in the Pappu Lab, received a travel award to attend the fourth biennial Intrinsically Disordered Proteins Gordon Research Conference held in Les Diabrelets, Switzerland in June 2016.
- Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab, received a travel award to attend the fourth biennial Intrinsically Disordered Proteins Gordon Research Conference held in Les Diabrelets, Switzerland in June 2016.
- 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 S. 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 S. 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 S. 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 S. 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 S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab gave an invited platform session talk at the 60<sup>th</sup> Annual Meeting of the Biophysical Society, February 2016.
- Mr. Tyler S. Harmon, Physics Graduate Student in the Pappu Lab gave an invited platform session talk at the 60<sup>th</sup> 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 M. 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, 59<sup>th</sup> 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 59<sup>th</sup> 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 3<sup>rd</sup> Gordon Research Conference on Intrinsically Disordered Proteins, Stonehill College, MA, June 2014.
- Mr. Albert H. Mao, MSTP and Computational & Molecular Biophysics Graduate Student in the Pappu Lab, received Washington University's Spencer T. Olin prize for outstanding graduate research, April 2014.
- Mr. Alex S. Holehouse, Computational & Molecular Biophysics Graduate Student in the Pappu Lab, Recipient of the SRAA Award for Best Poster, 58<sup>th</sup> 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 58<sup>th</sup> 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, 58<sup>th</sup> 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, 57<sup>th</sup> 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 56<sup>th</sup> 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, 5<sup>th</sup> Annual Symposium of the Intrinsically Disordered Proteins Subgroup at the 55<sup>th</sup> 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, 55<sup>th</sup> 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 54<sup>th</sup> 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 articles in press**

1. J. B. Warner IV<sup>§</sup>, K. M. Ruff<sup>§</sup>, P. S. Tan, E. A. Lemke, **R. V. Pappu\***, H. A. Lashuel\*. Monomeric huntingtin exon 1 has similar overall structural features for wild type and pathological polyglutamine length. (2017). (<sup>§</sup>Co-first authors, \*Co-corresponding authors). *Journal of the American Chemical Society, in press.* (<http://dx.doi.org/10.1021/jacs.7b06659>)
2. K. Sherry, R.K. Das, **R.V. Pappu\***, D. Barrick\*. Control of transcriptional activity through



- de novo* design of sequence-to-conformation relationships of the intrinsically disordered RAM region of the Notch intracellular domain. (2017). (\*Co-corresponding authors). *Proceedings of the National Academy of Sciences USA*, In press.
- G. Fuertes<sup>#</sup>, N. Banterle<sup>#</sup>, K.M. Ruff<sup>#</sup>, A. Chowdhury, D. Mercadante, C. Koehler, M. Kachala, G. E. Girona, S. Milles, A. Mishra, P. R. Onck, F. Gräter, S. Esteban-Martin, **R.V. Pappu**<sup>\*</sup>, D. I. Svergun<sup>\*</sup>, E. A. Lemke<sup>\*</sup> (<sup>#</sup>Co-first authors, <sup>\*</sup>Co-corresponding authors). Decoupling of size and shape fluctuations in heteropolymeric sequences reconciles discrepancies in SAXS versus FRET measurements. (2017). *Proceedings of the National Academy of Sciences USA*. **114**: E6342-E6351.
  - S. Chatterjee, P. Luthra, E. Esaulova, E. Agapov, B. Yen, D. Borek, M. Edwards, A. Mittal, D. Jordan, P. Ramanan, M. Moore, **R.V. Pappu**, M. Holtzman, M.N. Artyomov, C. Basler, G. Amarasinghe, and D. Leung (2017). Structural basis for human respiratory syncytial virus NS1-mediated modulation of host responses. *Nature Microbiology*, **2**: 17101(1-8).
  - M-T. Wei<sup>#</sup>, S. Elbaum-Garfinkle<sup>#</sup>, A.S. Holehouse<sup>#</sup>, C. C-H. Chen, M. Feric, C.B. Arnold, R. D. Priestly, **R.V. Pappu**<sup>\*</sup>, C.P. Brangwynne<sup>\*</sup>. (2017). Phase separation of intrinsically disordered proteins yields permeable, low-density liquid droplets. *Nature Chemistry*, <http://dx.doi.org/10.1038/nchem.2803>. (<sup>#</sup>Co-first authors, <sup>\*</sup>Co-corresponding authors).
  - J. Clarke, **R.V. Pappu**. Protein folding and binding, complexity comes of age. (2017). *Current Opinion in Structural Biology*, **42**: 5-7.
  - P. Sormanni, D. Piovesan, G. Heller, M. Bonomi, P. Kukic , C. Camilloni, M. Fuxreiter, Z. Dosztanyi , **R. Pappu**, M. M. Babu , S. Longhi , P. S. Tompa , A.K. Dunker , V.N. Uversky , S. Tosatto, M. Vendruscolo. (2017). Simultaneous quantification of protein order and disorder. *Nature Chemical Biology*, Commissioned Commentary, **13**: 339-342.
  - T.S. Harmon, A.S. Holehouse, **R.V. Pappu**. To mix, or to demix, that is the question. *Biophysical Journal*, **112**: 565-567, Invited New & Notable piece.
  - V. Kalas, J.S. Pinkner, T. J. Hannan, M. E. Hibbing, K. W. Dodson, A. S. Holehouse, H. Zhang, N. H. Tolia, M. L. Gross, **R. V. Pappu**, J. Janetka, S.J. Hultgren. (2017). Evolutionary fine-tuning of conformational ensembles in FimH during host-pathogen interactions. *Science Advances*. **3**: e1601944.
  - A. S. Holehouse<sup>\*</sup>, R.K. Das, J. Ahad, M. O. G. Richardson, **R.V. Pappu**<sup>\*</sup>. (2017). CIDER: Resources to analyze sequence-ensemble relationships of intrinsically disordered proteins. *Biophysical Journal*. **112**: 16-21 (\*Co-corresponding authors). **Selected and evaluated by Faculty of 1000**.
  - E.W. Martin<sup>†</sup>, A.S. Holehouse<sup>†</sup>, C.R. Grace, A. Hughes, **R.V. Pappu**<sup>\*</sup>, T. Mittag<sup>\*</sup>. (2016). Sequence determinants of the conformational properties of an intrinsically disordered protein prior to and upon phosphorylation. *Journal of the American Chemical Society* **138**: 15323-15335. (<sup>†</sup>Co-first authors; <sup>\*</sup>Co-corresponding authors).
  - T.S. Harmon, M.D. Crabtree, S.L. Shammass, 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*, **29**: 339-346. **Selected and evaluated by Faculty of 1000**.
  - C.W. Pak, M. Kosno, A.S. Holehouse, S. Padrick, A. Mittal, R. Ali, A. Yunus, D. R. Liu, **R.V. Pappu**<sup>\*</sup>, M.K. Rosen<sup>\*</sup>. (2016). Sequence determinants of intracellular phase separation via complex coacervation of a model disordered protein. *Molecular Cell*, **63**: 72-85. <sup>\*</sup>Co-corresponding authors.

14. 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.
15. R.K. Das, Y. Huang, A. Phillips, R.W. Kriwacki, **R.V. Pappu**. (2016). Cryptic sequence features within the disordered protein p27<sup>Kip1</sup> regulate cell cycle signaling. *Proceedings of the National Academy of Sciences USA*. **113**: 5616-5621.
16. 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.
17. K.M. Ruff, T.S. Harmon, **R.V. Pappu**. (2015). CAMELOT: A machine learning optimized approach for coarse-grained simulations aggregation of block-copolymeric protein sequences. *Journal of Chemical Physics*. **143**: 243123.
18. C.P. Brangwynne, P.S. Tompa, **R.V. Pappu**. (2015). Polymer Physics of Intracellular Phase Transitions. *Nature Physics*. **11**: 899-904.
19. A.S. Holehouse, **R.V. Pappu**. Encoding phase transitions. (2015). *Nature Materials*. **14**: 1083-1084. Invited News & Views piece.
20. 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.
21. 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.
22. 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.
23. **R.V. Pappu** (2015). Cell signaling, division, and organization mediated by intrinsically disordered proteins. *Seminars in Cell and Developmental Biology*. **37**: 1-2.
24. 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.
25. 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.
26. 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**.
27. 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.
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### Submitted Manuscripts

1. I. Peran, A.S. Holehouse, S. V. Kathuria, **R.V. Pappu**, I. S. Carrico, O. Bilsel, D. P. Raleigh. Direct Observation of a Protein Collapse Transition: A High Efficiency Bio-orthogonal Labeling Strategy Facilitates Studies of Protein Unfolded States. (2017). *Journal of the American Chemical Society*, revised version under review.
2. T.S. Harmon, A.S. Holehouse, M.K. Rosen, **R.V. Pappu**. Intrinsically disordered linkers determine the interplay between phase separation and gelation in multivalent proteins. *eLife*, revised version being prepared for submission following first round of reviews. **Preprint:** <http://www.biorxiv.org/content/early/2017/07/16/164301>.
3. T. M. Franzmann, M. Jahnel, A. Pozniakovsky, J. Mahamid, A.S. Holehouse, E. Nüske, D. Richter, W. Baumeister, S.W. Grill, **R.V. Pappu**, A.A. Hyman, S. Alberti. A prion domain that promotes cellular fitness by pH regulated phase separation. *Science*, revised version being prepared for submission following first round of reviews.
4. L-P Bergeron-Sandoval, H. Khadivi Heris, A. G. Hendricks, A. J. Ehrlicher, P. François, **R. V. Pappu**, S. W. Michnick. Endocytosis caused by liquid-liquid phase separation of proteins. (2017). *Nature*, revised version being prepared for submission following first round of reviews. **Preprint:** <http://www.biorxiv.org/content/early/2017/06/23/145664>.
5. J. Fei\*, M. Jadalih<sup>§</sup>, T. S. Harmon<sup>§</sup>, I.T.S. Li, B. Hua, A. S. Holehouse, M. Reyer, Q. Sun, S. M. Freier, **R. V. Pappu**, K. V. Prasanth\*, T.J. Ha. Proteins and RNAs display multilayer organization in nuclear speckles. (2017). (\*co-corresponding authors; <sup>§</sup>equal contributors). *Journal of Cell Science*, revised version being prepared for submission following first round of reviews.
6. S. Roberts, J. Schaal, T. S. Harmon, K. Li, A. Hunt, V. Miao, Y. Wen, T. G. Oas, J. Collier, **R. V. Pappu**, A. Chilkoti. Modulation of order and disorder in recombinant polypeptides creates injectable tissue integrating networks. *Nature Materials*, revised version being prepared for submission following first round of reviews.

7. H. Mirbaha, O.A. Morozova, K.M. Ruff, A. Sharma, R.V. Pappu, D.W. Colby, H. Mirzai, L.A. Jochimiak, M.I. Diamond. Inert and seed-competent tau monomers elucidate the structural origins of aggregation. *eLife*, under review. **Preprint:** <http://www.biorxiv.org/content/early/2017/07/14/163394>.
8. M.V. Staller, A.S. Holehouse, D. Swain-Lenz, R.K. Das, **R.V. Pappu**, B.A. Cohen. Design principles of an acidic activation domain. *Cell Systems*, under review.
9. A.S. Holehouse, **R.V. Pappu**. Collapse transitions of proteins and the interplay amongst polypeptide backbone, sidechain and solvent interactions. *Invited contribution submitted to Annual Review of Biophysics*.
10. A.E. Posey, K.M. Ruff, T.S. Harmon, S.L. Crick, Z. Zheng, A. Li, M.I. Diamond, **R.V. Pappu**. Profilin binding modulates aggregation and phase separation of huntingtin N-terminal fragments via polyphasic linkage. *Submitted to Proceedings of the National Academy of Sciences USA*.

### **Manuscripts in preparation**

1. S.K. Powers, A.S. Holehouse, D.A. Korasick, K.H. Schreiber, E. Tycksen, J.M. Jez, **R.V. Pappu**, L.C. Strader. Nucleo-cytoplasmic partitioning of ARF proteins control auxin responses in *Arabidopsis thaliana*.
2. E. A. Newcombe<sup>§</sup>, K. M. Ruff<sup>§</sup>, Y. M. Ramdzan, A. Sethi, A. R. Ormsby, O. Kleifeld, A. W. Purcell, P. R. Gooley, **R. V. Pappu**<sup>\*</sup>, D. M. Hatters<sup>\*</sup>. (<sup>§</sup>Co-first authors, <sup>\*</sup>Co-corresponding authors). Tadpole-like conformations of huntingtin exon 1 with expanded polyglutamine engender novel interactions in cells. **Preprint:** <http://www.biorxiv.org/content/early/2017/08/22/179663>
3. M. C. Cohan, A.E. Posey, A. Mittal, S. Grigsby, J. Lalmansingh, A.S. Holehouse, P. A. Levin, **R.V. Pappu**. How does the C-terminal intrinsically disordered tail of FtsZ impact self-assembly and cell division in rod-shaped bacteria?
4. 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 Aβ oligomers. *To be submitted to special issue of Protein Science on protein aggregation*.
5. A. Mittal, A.S. Holehouse, **R.V. Pappu**. Bristles and linkers: Sequence-specific conformational properties of intrinsically disordered regions tethered to folded domains of proteins. *To be submitted to special issue of Journal of Molecular Biology on intrinsically disordered proteins*.
6. T.S. Harmon, S. Roberts, A. Chilkoti, **R.V. Pappu**. Physical model for programmable hysteresis in partially ordered protein polymers that undergo thermoresponsive phase transitions. *To be submitted to special issue of Journal of Molecular Biology on Phase Separation of Intrinsically Disordered Proteins*.
7. T.S. Harmon, A.S. Holehouse, **R.V. Pappu**. Differential solvation of intrinsically disordered linkers linear multivalent proteins can lead to spatially organized droplets. *To be submitted to special issue of New Journal of Physics on Membraneless Organelles*.
8. S. Barrera-Vilarmau<sup>\*</sup>, A.S. Holehouse<sup>\*</sup>, L. Chemes, **R.V. Pappu**. Physico-chemical principles underlying the conservation of sequence-ensemble relationships in rapidly evolving intrinsically disordered proteins. *Invited feature article to be submitted to Journal of Physical Chemistry B*. (<sup>\*</sup>Co-first authors).
9. I. Peran<sup>\*</sup>, A.S. Holehouse<sup>\*</sup>, I.S. Caricco, **R.V. Pappu**, O. Bilsel, D.P. Raleigh. Direct



observation of protein collapse transitions and characterization of unfolded states under folding conditions. (\*Co-first authors).

10. A.S. Holehouse, **R.V. Pappu**. Functional implications of phase transitions in cell biology. *Invited perspective for Biochemistry special issue on membraneless organelles*.
11. A.S. Holehouse, **R.V. Pappu**. PIMMS: A novel lattice-based approach for modeling the sequence-encoded phase behavior of intrinsically disordered proteins.
12. T.S. Harmon\*, A.E. Posey\*, **R.V. Pappu**. Preferential charge neutralization stabilizes alpha helices in peptides with specific patterns of oppositely charged residues.
13. K.M. Ruff, **R.V. Pappu**. Computational methods for multiscale simulations of intrinsically disordered proteins. *Invited review in preparation for Quarterly Reviews in Biophysics*.
14. A.S. Holehouse, T.S. Harmon, C.P. Brangwynne, **R.V. Pappu**. Biophysical principles underlying the phase transitions of multivalent and intrinsically disordered proteins. *Invited review in preparation for Biophysical Journal*.
15. J.M. Choi, **R.V. Pappu**. Improvements to the ABSINTH implicit solvation model and forcefield paradigm based on a refined coil library.
16. J.M. Choi, J. Lalmansingh, K. Bharath, **R.V. Pappu**. Comparative assessments of molecular mechanics forcefields against a refined statistical coil library for peptides.

## Grants

### CURRENT

#### National Science Foundation – DMREF Collaborative Research

**Title:** *High throughput exploration of sequence space of peptide polymers that exhibit aqueous demixing phase behavior*

**Funding Period:** October 01, 2017 – September 30, 2021

**Principal Investigator:** Ashutosh Chilkoti, Duke University

**Role in the project:** *Co-Principal Investigator* with Stefan Zauscher (Duke University)

#### Human Frontier Science Program (HFSP)

**Title:** *Elucidating the molecular logic of membrane-free compartment function and assembly*

**Funding period:** September 01, 2017 – August 31, 2020

**Role in the project:** *Co-Principal Investigator* with Simon Alberti (Max Planck Institute, Dresden) and Stephen W. Michnick (University of Montreal)

**St. Jude Research Collaborative**, Sponsored by St. Jude Children’s Research Hospital,

**Title:** *Biology and Biophysics of Membraneless Organelles*

**Funding period:** February 01, 2017 – January 31, 2022

**Role in the project:** *Project Principal Investigator*, Computational & Theoretical Modeling

#### National Science Foundation, MCB-1614766

**Title:** *Multiscale Modeling of Phase Transitions Driven by Multivalency and Disordered Proteins*

**Funding period:** July 15, 2016 – July 14, 2020

**Role in the project:** *Principal Investigator*

#### 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:** *Principal Investigator*

**National Institutes of Health, 1R01NS089932-A1**

**Title:** *Mechanism of modulation of huntingtin exon 1 aggregation by profilin*

**Funding period:** April 01, 2016 – March 31, 2021

**Principal Investigators:** Rohit Pappu (contact PI), Marc I. Diamond, and Ralf Langen

**Role in the project:** *Main Principal Investigator* in Multi-PI grant

**National Institutes of Health, 1R01GM108785**

**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*

## PENDING

**National Institutes of Health RO1NS105497**

**Title:** *Huntingtin Conformation and Neurodegeneration*

**Proposed Funding Period:** January 01, 2018 – December 31, 2022

**Principal Investigator:** Steven Finkbeiner, UCSF and the Gladstone Institute

**Role in the project:** *Co-Principal Investigator* in Multi-PI proposal

## 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 A $\beta$  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 and localCIDER – 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 our 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 is the main developer of CIDER. Available for free download from <http://pappulab.github.io/localCIDER/>.
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. **Furquan Dar**, Doctoral Student, Department of Physics, Projected graduation date, December 2021.
3. **Kourtney Kroll**, Undergraduate researcher, Senior in Biomedical Engineering, Washington University in St. Louis.

4. **Jared Lalmansingh**, Doctoral Student, Department of Physics. Projected graduation date, December 2020.
5. **Divya Natarajan**, MD Student, Washington University School of Medicine, graduation date, May 2020.

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

1. **Jeong-Mo Choi**, Postdoctoral Scientist
2. **Martin Fossat**, Postdoctoral Scientist
3. **Alex S. Holehouse**, Postdoctoral Scientist
4. **Sang Eun Jee**, Postdoctoral Scientist
5. **Ammon E. Posey**, Research Scientist
6. **Mary O. G. Richardson**, Junior Research Scientist and Scientific Programmer
7. **Kiersten M. Ruff**, Postdoctoral Scientist

***Lab alumni – reverse chronological order***

1. **Tyler S. Harmon**, Doctoral Student, Department of Physics. Received PhD in April 2017. Currently, postdoctoral scientist at the Max Planck Institute in Dresden, Germany.
2. **Rajni Verma**, Postdoctoral Scientist, October 2015 – May 2016.
3. **Rahul K. Das**, Postdoctoral Scientist. Currently, a senior research scientist at GNS Healthcare, Cambridge, MA.
4. **Anuradha Mittal**, Postdoctoral Scientist. Currently, a senior Bioinformatics Scientist at Affymetrix, San Francisco, CA.
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. University of California, Berkeley, Molecular and Cell Biology, April 2017
2. Hospital for Sick Kids, Toronto, Molecular Medicine Seminar Series, March 2017
3. Washington University, Department of Genetics Seminar Series, February 2017
4. McGill University, Department of Biology, January 2017
5. Princeton University, Department of Chemical & Biochemical Engineering, December 2016
6. Tata Institute for Fundamental Research, Mumbai, India, November 2016
7. Department of Biomedical Engineering, Washington University in St. Louis, October 2016
8. MRC Laboratory of Molecular Biology, Cambridge, UK, June 2016
9. Johns Hopkins University, Department of Materials Science, April 2016
10. Hiroshima University, December 2015
11. Duke University, NSF-MRSEC, April 2015
12. University of British Columbia, Center for High-Throughput Biology, April 2015
13. Washington University in St. Louis, Biophysical Evening, January 2015
14. University of Texas Southwestern Medical Center, Department of Biophysics, December 2014
15. University of Cambridge, Department of Chemistry, November 2014
16. MRC Laboratory of Molecular Biology, Cambridge, UK, November 2014
17. Stony Brook University, Laufer Center for Quantitative Biology, November 2014
18. Kansas State University, Department of Biochemistry, April 2014
19. Ohio State University, Department of Biochemistry, Biophysics Program, April 2014
20. University of Montana, Department of Chemistry & Biochemistry, February 2014
21. Johns Hopkins University, Department of Biophysics, December 2013
22. University of Wisconsin-Madison, Department of Chemical & Biochemical Engineering, December 2013
23. University of Zurich, Department of Biochemistry, September 2013
24. The Scripps Research Institute, Department of Molecular & Experimental Medicine, July 2013
25. University of Texas Southwestern Medical Center, University Colloquium, July 2013
26. University of Texas Southwestern Medical Center, Green Center for Systems Biology, Special Seminar, July 2013
27. Symposium on Physics and Biology of Strongly Fluctuating Proteins, University of Maryland, May 2013
28. American Chemical Society Meeting, New Orleans, April 2013
29. University of Chicago, Institute for Biophysical Dynamics, April 2013
30. March Meeting of the American Physical Society, Baltimore, March 2013
31. CUNY City College of New York, Structural Biology Colloquium, March 2013
32. 57<sup>th</sup> Annual Meeting of the Biophysical Society, Philadelphia, Protein Electrostatics Symposium
33. University of Minnesota, Department of Biomedical Engineering, December 2012

34. Protein Folding Consortium, Pls meeting, Chicago, November 2012
35. International Symposium on Protein Folding, National Centre for Biological Sciences, Bangalore, India, October 2012
36. Protein Folding Consortium, SUNY Stony Brook, NY, June 2012
37. Biopolymers Gordon Research Conference, Newport, RI, June 2012
38. Hope Center for Neurological Disorders, Washington University, May 2012
39. Arizona State University, Center for Biological Physics, Tempe, AZ, April 2012
40. University of South Florida, Department of Physics, Tampa, FL, March 2012
41. St. Jude Children's Research Hospital, Memphis, TN, January 2012
42. CCP 2011 – Conference on Computational Physics, Knoxville, TN, November 2011
43. National Science Foundation Workshop on Future of RNA and Protein Folding, Arlington, VA, September 2011
44. University of Leeds, UK, July 2011
45. MRC Laboratory of Molecular Biology, Cambridge, UK, July 2011
46. Annual Meeting of the Protein Folding Consortium, UC Berkeley, June 2011
47. University of Texas Southwestern Medical School, May 2011
48. The Scripps Research Institute, Molecular & Experimental Medicine, May 2011
49. Washington University School of Medicine, Computational & Molecular Biophysics Program, Biophysical Evening Series, May 2011
50. Midwest Conference on Protein Folding, Assembly, and Molecular Motions, May 2011
51. 55<sup>th</sup> Annual Meeting of the Biophysical Society, Baltimore, MD, March 2011
52. Department of Biochemistry, Cornell Weill Medical College, December 2010
53. ACS Midwest Regional Meeting Symposium on Protein Folding, October, 2010
54. Intrinsically disordered proteins, Keynote Session Chair, Gordon Research Conference, North Carolina, July 2010.
55. Protein folding pathways workshop, Arizona State University, May 2010.
56. University of Pittsburgh School of Medicine, March 2010.
57. Yale University, Biophysics program, January 2010.
58. Protein folding and dynamics, Gordon Research Conference, January 2010.
59. The Scripps Research Institute, Molecular & Experimental Medicine, November 2009.
60. 23<sup>rd</sup> Annual Gibbs conference on Biothermodynamics, Carbondale, IL, October 2009.
61. Tata Institute of Fundamental Research, Mumbai, India, August 2009.
62. Argonne National Laboratory, Biology Division, August 2009.
63. Northwestern University, Biochemistry, Molecular Biology & Cell Biology, July 2009.
64. Telluride Scientific Research Conference, Workshop on RNA dynamics, July 2009.
65. FASEB Amyloid meeting, Snowmass, CO, June-July 2009.
66. University of California Berkeley, Department of Bioengineering, April 2009.
67. MIT-Whitehead Institute, Department of Biology, March 2009.
68. Annual Meeting of the Biophysical Society, Invited Workshop, Boston, MA, March 2009.
69. Department of Chemistry & Biochemistry, University of Massachusetts, Amherst, MA, February 2009
70. Rice University, Department of Chemistry, November 2009.
71. Rensselaer Polytechnic Institute, Biocomputation seminar series, October 2008.
72. 22<sup>nd</sup> Annual Symposium of the Protein Society, July 2008, San Diego, CA
73. Protein Electrostatics Workshop, Telluride, CO, July 2008



74. Biopolymers Gordon Research Conference, Newport, RI, June 2008.
75. University of Texas Austin, Department of Biomedical Engineering, April 2008.
76. University of Oregon, Department of Chemistry, April 2008.
77. Intrinsically Disordered Proteins subgroup meeting, Annual meeting of the Biophysical Society, Long Beach, CA, February 2008
78. The Scripps Research Institute, Department of Chemistry, La Jolla, CA, September 2007.
79. Gordon Research Conference: Proteins, June 2007, Holderness, New Hampshire.
80. Washington University in St. Louis, Biophysical Evening Series, December 2007.
81. University of California in Santa Barbara, Department of Chemistry, April 2007.
82. University of Delaware, Department of Chemistry and Biochemistry, April 2007.
83. Indiana University, Computational Biology and Bioinformatics, September 2006.
84. National Cancer Institute, Frederick, August 2006.
85. FASEB Amyloid Meeting, Snowmass, Colorado, June 2006.
86. DIMACS Workshop on Computational / Experimental Approaches to Protein Defects in Human Disease, Rutgers University, April 2006.
87. University of North Carolina, Chapel Hill, Department of Chemistry, April 2006.
88. Duke University, Department of Biochemistry, April 2006.
89. UTMB, Galveston, TX, Sealy Center for Structural Biology, April 2006.
90. Johns Hopkins University, Department of Chemistry, March 2006.
91. Stanford University, Department of Chemistry, March 2006.
92. I2CAM Exploratory Workshop on Protein Aggregation and Amyloid Formation in Systemic and Neurodegenerative Diseases: Physical, Molecular, and Biological Approaches, EPFL, Lausanne, Switzerland, July 2005.
93. 18<sup>th</sup> Annual Gibbs Conference on Biothermodynamics, Carbondale IL, October 2004.
94. University of Iowa, Department of Chemistry, Iowa City, May 2004.
95. Washington University, Alzheimer's disease Research Center, April 2004.
96. Washington University, Department of Genetics, October 2002.
97. Washington University, Alzheimer's disease Research Center, December 2002.
98. Washington University, Biophysical Evening Seminar Series, December 2001.

## TEACHING

1. *Bioengineering Thermodynamics in Practice*, Laboratory Course, BME 329, Fall 2014 & 2015. Audience: Biomedical Engineering juniors.
2. *Bioengineering Thermodynamics*, BME 320B, Fall 2010 onward. Audience: Biomedical Engineering juniors.
3. *Applied Mathematics for Biomedical Sciences*, Fall 2013. Audience: Graduate students in Biomedical Engineering & quantitative programs in the Division of Biology & Biomedical Sciences.
4. *Chemical Thermodynamics*, ChemE 320 / BME 320, Fall 2008 and 2009. Audience: Chemical Engineering sophomores and Biomedical Engineering juniors.
5. *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.

6. *Principles of Protein Structure, BME 461*, Every Fall starting Fall 2003. Audience: Seniors and graduate students in Biomedical Engineering.
7. *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.
8. *Modeling Biomolecular Systems, Part II, BME 540*, Fall 2004. Audience: Graduate students in Biomedical Engineering, Chemical Engineering, Molecular Biophysics, and Computational Biology.
9. *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.
10. *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 currently co-chairing the strategic planning committee commissioned by the Dean of the School of Engineering & Applied Sciences. The goal is to craft a strategic plan for the next 5-10 year period for the school.

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 1<sup>st</sup> 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 20<sup>th</sup> Annual Gibbs Meeting on Biothermodynamics, October 7-10, 2006, Carbondale, IL.