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PROFESSIONAL BACKGROUND

Academic Positions

January 2019 - current: Director of CSELS, Center for the Science and Engineering of Living Systems, Washington University in St. Louis

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

September 2012 – December 2018: Director, Center for Biological Systems Engineering, Washington University in St. Louis, School of Engineering & Applied Sciences

January 2013 – January 2018: Co-Director, Center for High Performance Computing, Washington University in St. Louis

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

Non-academic Affiliations

January 2019 - current: Member, Scientific Advisory Board, Dewpoint Therapeutics, Boston, MA and Dresden, Germany

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 are actively working on 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. Specific foci include nuclear bodies, stress responses, synaptic bodies, and the interplay between spontaneous and driven processes.

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.

Honors and Awards

Invited Keynote Speaker, Gordon Research Conference on Computational Aspects of Biomolecular NMR, Les Diablerets, Switzerland, June 2019

Invited Closing Keynote Speaker for Gordon Research Seminar on Computational Aspects of Biomolecular NMR, Les Diablerets, Switzerland, June 2019

Named as **Mercator Fellow** by the Deutsche Forschungsgemeinschaft (German Research Foundation) to serve as an international collaborator with Professor Dr. **Edward A. Lemke** (Adjunct Director, Institute of Molecular Biology, and Professor of Synthetic Biophysics, Johannes Gutenberg University, Mainz), Professor Dr. **Simon Alberti** (Professor of Cellular Biochemistry, Technische Universität Dresden, Center for Molecular and Cellular Bioengineering and Biotechnology Center (BIOTEC)), and Professor Dr. **Claus A.M. Seidel** (Chair of Molecular Physical Chemistry, Heinrich Heine University Düsseldorf). The three-year fellowship, starting in 2019, funds visits to Germany and enables the 4-way investigations focused on the internal structure and related proteins in stress granules.

Elected as **Fellow** of the US **Biophysical Society**, 2019

Invited participant and speaker in the Banbury Center meeting on Phase Separated Assemblies in Cell Biology, Cold Spring Harbor Laboratory, December 16-19, 2018

Invited Keynote Speaker, Dutch Biophysical Society, Veldhoven, Netherlands, October 2018

Co-Chair of NIH ZRG1-MDCN study section, July 2018

Member, Scientific Advisory Board at the Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany, term ending December 31, 2022

Chair the 2017 FASEB Summer Research Conference on Molecular Mechanisms and Physiological Consequences of Protein Aggregation

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.

Guest Editor, Current Opinion in Structural Biology, 2017

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

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

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

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

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

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

Invited Talks at National and International Conferences / Symposia / Workshops

Invited Speaker, EMBO workshop on *Transcription in Yeast*, Girona, Spain, June 2020

Invited Speaker, Royal Society of Chemistry sponsored workshop on *Anhydrous Proteins*, Chichley Hall, Buckinghamshire, UK, March 2020

Invited Speaker, International Conference on *Applied Bioinformatics in Living Systems*, Leuven, Belgium, February 2020

Invited Speaker, EMBO workshop on *Intrinsically Disordered Proteins: From Molecules to Systems*, Bangalore, India, December 2019

Invited Speaker, Telluride Science Research Conference on *Intrinsically Disordered Proteins*, July 2019

Invited Speaker, National Cancer Institute strategic workshop on *Liquid phase separation as a cellular regulatory mechanism: State of the science and implications for cancer research*, Bethesda, MD, May 2019

Invited Speaker, *Cell Press Symposium on Regulatory RNAs*, Berlin, Germany, May 2019

Invited Speaker, Keystone Symposium on *Biomolecular Condensates: Phase separated organizers of cellular biochemistry*, Snowbird, Utah, April 2019

Invited Symposium Speaker, 63rd Annual Meeting of the Biophysical Society, Baltimore, March 2019

Invited Speaker, *Symposium on Phase Separation in Biology and Disease*, New York Academy of Sciences, February 2019

Invited Speaker, *workshop on Phase Transitions in Polymeric and Protein Systems*, Organized by the Max Planck Institute for Physics of Complex Systems, Dresden, Germany, February 2019

Invited Lecturer, *EMBO course on Phase Transitions in Polymeric and Protein Systems*, Organized by the Max Planck Institute for Cell Biology & Genetics, Dresden, Germany, February 2019

Invited Speaker, 2019 *BMES Cellular and Molecular Bioengineering Conference*, San Diego, CA, January 2019

Invited Speaker and Session Chair, *Intrinsically Disordered Proteins Gordon Research Conference*, Les Diablerets, Switzerland, July 2018

Invited Speaker, *EMBO | EMBL Symposium: Cellular Mechanisms Driven by Liquid Phase Separation*, Heidelberg, Germany, May 2018

Invited Speaker, *ASBMB Symposium at Experimental Biology*, San Diego, CA, April 2018

Invited Speaker, 13th *CHDI Annual Huntington's Disease Therapeutics Conference: A forum for Drug Discovery and Development*, Palm Springs, CA, February 2018

Invited Speaker, *International Conference on Intrinsically Disordered Proteins*, IISER Mohali, India, December 2017

Invited Speaker, Build the Cell Subgroup Symposium at the Annual Meeting of the American Society for Cell Biology, Philadelphia, PA, December 2017

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

Keynote Distinguished Speaker, Syracuse Biomaterials Institute, Syracuse University, April 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 253rd National Meeting of the American Chemical Society, San Francisco, April 2017

Invited Speaker, 3rd International Workshop on Protein Folding & Dynamics, National Centre for Biological Sciences, Bangalore, 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

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

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

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

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

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

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

Dr. Alex S. Holehouse, postdoc in the Pappu lab, received the 2019 MolSSI "seed" software fellowship from the Molecular Sciences and Software Institute to develop a computational pipeline for modeling the evolution and sequence-ensemble relationships of intrinsically disordered proteins.

Dr. Max Staller, joint postdoc in the Cohen and Pappu labs, was chosen to give two lectures as part of the Gene Regulatory Networks in Development course at the Molecular Biology Laboratory in Woods Hole, MA in October 2018.

Mr. Conor O'Neill, first year Biomedical Engineering graduate student in the Pappu lab, was matched with the Kent and Bonnie Lattig fellowship in the Center for Biological Systems Engineering at Washington University in St. Louis for the 2018-2019 academic year.

Dr. Alex S. Holehouse, postdoctoral fellow in the Pappu lab, received an award for one of the three best posters presented by postdocs at the 2018 Gordon Research Conference on Intrinsically Disordered Proteins held in Les Diablerets, Switzerland.

Ms. Megan C. Cohan, graduate student in the Pappu lab, was elected by her peers to co-chair the 2020 Gordon Research Seminar that will precede the 2020 Gordon Research Conference on Intrinsically Disordered Proteins.

Dr. Kiersten M. Ruff, postdoctoral fellow in the Pappu lab, was chosen to give a special talk at the 2018 Gordon Research Conference on Intrinsically Disordered Proteins held in Les Diablerets, Switzerland.

Ms. Megan C. Cohan, graduate student in the Pappu lab, was chosen to speak at the 2018 Gordon Research Seminar (GRS) that preceded the 2018 Gordon Research Conference on Intrinsically Disordered Proteins in Les Diablerets, Switzerland, July 2018.

Ms. Megan C. Cohan, graduate student in the Pappu lab, was chosen to receive a travel award, based on her submitted abstract, to present a poster at the EMBO | EMBL Symposium on Cellular Mechanisms Driven by Liquid Phase Separation, May, 2018.

Dr. Kiersten M. Ruff, postdoctoral fellow in the Pappu lab, was chosen, based on her submitted abstract, to speak at the EMBO | EMBL Symposium on Cellular Mechanisms Driven by Liquid Phase Separation, May, 2018.

Ms. Mary O.G. Richardson, scientific programmer and junior research scientist in the Pappu lab received the prestigious NSF graduate student fellowship for her PhD studies in Computational Biology.

Dr. Jeong-Mo Choi, postdoctoral fellow in the Pappu lab, was chosen to speak in a platform session on intrinsically disordered proteins at the 62nd Annual Meeting of the Biophysical Society, San Francisco, February 2018.

Dr. Kiersten M. Ruff, postdoctoral fellow in the Pappu lab, was chosen to speak in a platform session on intrinsically disordered proteins at the 62nd Annual Meeting of the Biophysical Society, San Francisco, February 2018.

Dr. Jeong-Mo Choi, postdoctoral fellow in the Pappu lab, was chosen to give the Molecular Kinetics sponsored postdoctoral talk at the 2018 symposium of the Intrinsically Disordered Proteins subgroup to be held in conjunction with the 62nd Annual Meeting of the Biophysical Society, San Francisco, February 2018.

Dr. Alex S. Holehouse, postdoctoral fellow in the Pappu lab, was one of the invited speakers in the symposium organized by the Biopolymers In Vivo Subgroup at 62nd Annual Meeting of the Biophysical Society, San Francisco, February 2018.

Dr. Alex S. Holehouse, postdoctoral fellow in the Pappu lab, was chosen to give a short talk at the 2018 Protein Folding Dynamics Gordon Research Conference, Galveston, TX, January 2018.

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.

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 given a student talk at the annual meeting of the NSF sponsored Protein Folding Consortium in Berkeley, CA, June 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, 61st 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 61st 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 23rd 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 Diablerets, 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 Diablerets, 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 Diablerets, 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 Diablerets, Switzerland, June 2016.

Mr. Alex S. 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 S. 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 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, 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. 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, 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 articles in press* (Google scholar h-index: 45; i10 index 84)**

1. S. Boeynaems†, A.S. Holehouse, V. Weinhardt, D. Kovacs, J. Van Lindt, C. Larabell, L. Van Den Bosch, R. Das, P. Tompa, **R.V. Pappu†,** A. Gitler†. (2019). Spontaneous driving forces give rise to protein-RNA condensates with coexisting phases and complex material properties. *Proceedings of the National Academy of Sciences USA, in press.* (†Co-corresponding authors).
2. R. Beveridge*, L G. Migas*, R. K. Das, **R. V. Pappu**, R. W. Kriwacki, P. E. Barran. (2019). Ion mobility mass spectrometry helps uncover the impact of charge patterning on the conformational distributions of intrinsically disordered proteins. (*Co-first authors). *Journal of the American Chemical Society, in press.*
3. J-M. Choi, **R.V. Pappu**. (2019). Improvements to the ABSINTH forcefield for proteins based on experimentally derived amino-acid specific backbone conformational statistics. *Journal of Chemical Theory and Computation,* **15**: 1367-1382.
4. J-M. Choi, **R.V. Pappu**. (2019). Experimentally derived and computationally optimized conformational statistics for blocked amino acids. *Journal of Chemical Theory and Computation*, **15**: 1355-1366.
5. K. M. Ruff*, **R.V. Pappu***, A.S. Holehouse*. (2019). Conformational preferences and phase behavior of low complexity sequences: Insights from multiscale simulations. *Current Opinion in Structural Biology,* **56:** 1-10. (*Co-corresponding authors).
6. A.E. Posey†, A.S. Holehouse†, **R.V. Pappu**. (2018). Phase separation of intrinsically disordered proteins. *Methods in Enzymology,* **611:** 1-30. (†Co-first authors).
7. S. Roberts, T. S. Harmon, J. Schaal, K. Li, A. Hunt, V. Miao, Y. Wen, T. G. Oas, J. Collier, **R. V. Pappu**, A. Chilkoti. (2018). Modulation of order and disorder in recombinant polypeptides creates injectable tissue integrating networks. *Nature Materials,* **17**: 1154–1163. **In the news:** https://pratt.duke.edu/about/news/biomaterials-frankenstein-proteins-help-heal-tissue
8. G. Fuertes, N. Banterle, K.M. Ruff, A. Chowdhury, **R.V. Pappu***, D. I. Svergun*, E.A. Lemke*. (2018). Comment on "Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water." *Science*, **361:** eaau8230. Technical comment solicited by the editors. (*Co-corresponding authors).
9. T.Y. Yoo, J-M. Choi, W. Conway, C-H. Yu, **R.V. Pappu**, D.J. Needleman. (2018). Measuring NDC80 binding reveals molecular basis of tension-dependent kinetochore-microtubule attachments. *eLife,* **7:** e36392.

10. K.M. Ruff, S. Roberts, A. Chilkoti*, **R.V. Pappu***. (2018). Advances in understanding stimulus responsive phase behavior of intrinsically disordered protein polymers. *Journal of Molecular Biology.* **430**: 4619-4635. (*Co-corresponding authors)
11. A.E. Posey, **R.V. Pappu**. (2018). A first glimpse of nucleation of phase transitions in living cells. (*Invited preview*). *Molecular Cell,* **71:** 1-3.
12. J. Wang, J-M. Choi, A.S. Holehouse, X. Zhang, M. Jahnel, S. Maharana, R. Lemaitre, A. Pozniakovski, D. Drechsel, I. Poser, **R. V. Pappu**, S. Alberti, A. A. Hyman. (2018). A molecular grammar underlying the driving forces for phase separation of prion-like RNA binding proteins. *Cell*, **174:** 688-699. **In the news:** https://www.mpi-cbg.de/news-events/latest-news/article/news/uncovering-molecular-grammar/ and https://bme.wustl.edu/Pages/news.aspx?newsid=889/).
13. H. Mirbaha, D. Chen, O.A. Morozova, K.M. Ruff, A. Sharma, X. Liu, M. Goodarzi, **R.V. Pappu**, D.W. Colby, H. Mirzai, L.A. Jochimiak, M.I. Diamond. (2018). Inert and seed-competent tau monomers elucidate the structural origins of aggregation. *eLife*, **7**: e36584.
14. A. Mittal, A.S. Holehouse, M.C. Cohan, **R.V. Pappu**. (2018). Sequence-to-conformation relationships of disordered regions tethered to folded domains of proteins. *Journal of Molecular Biology,* **430:** 2403-2421.
15. E. A. Newcombe[§], K. M. Ruff[§], Y. M. Ramdzan, A. Sethi, A. R. Ormsby, O. Kleifeld, A. W. Purcell, P. R. Gooley, **R. V. Pappu**[*], D. M. Hatters[*]. (2018). Tadpole-like conformations of huntingtin exon 1 are characterized by conformational heterogeneity that persists for wild type and pathogenic polyglutamine lengths. ([§]Co-first authors, [*]Co-corresponding authors). *Journal of Molecular Biology,* **430**: 1442-1458.
16. T.S. Harmon, A.S. Holehouse, **R.V. Pappu.** (2018). Differential solvation of intrinsically disordered linkers drives the formation of spatially organized droplets in ternary systems of linear multivalent proteins. *New Journal of Physics*, **20:** 045002.
17. K. Garai, A.E. Posey, X. Li, E.M. Powers, J. Buxbaum, **R.V. Pappu**. (2018). Inhibition of amyloid beta fibril formation by monomeric human Transthyretin. *Protein Science,* **27:** 1252-1261.
18. M.V. Staller, A.S. Holehouse, D. Swain-Lenz, R.K. Das, **R.V. Pappu**, B.A. Cohen. (2018). A high-throughput mutational scan of an intrinsically disordered acidic transactivation domain. *Cell Systems,* **6**: 444-455.e6.
19. A.E. Posey, K.M. Ruff, T.S. Harmon, S.L. Crick, A. Li, M.I. Diamond, **R.V. Pappu**. (2018). Profilin reduces aggregation and phase separation of huntingtin N-terminal fragments by preferentially binding to soluble monomers and oligomers. *Journal of Biological Chemistry*, **293:** 3734-3746. (**Article selected to be part of the JBC special issue on Amyloids, Prions, and Oligomers** - http://www.jbc.org/site/vi/amyloids/)
20. A.S. Holehouse, **R.V. Pappu**. (2018). Collapse transitions of proteins and the interplay amongst polypeptide backbone, sidechain, and solvent interactions. *Annual Review of Biophysics,* **47:** 19-39.
21. A.S. Holehouse, **R.V. Pappu**. (2018). Functional implications of intracellular phase transitions. *Biochemistry,* **57**: 2415-2423.
22. 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. (2018). Phase separation by a yeast prion protein promotes cellular fitness. *Science,* **359**: eaao5654. **In the news:** https://www.mpi-cbg.de/press/press-releases/article/news/the-bright-side-of-an-

infectious-protein/.

23. J. Fei*, M. Jadalih[§], T. S. Harmon[§], I.T.S. Li, B. Hua, A. S. Holehouse, M. Reyer, Q. Sun, S. M. Freier, **R. V. Pappu**, K. V. Prasanth*, TJ. Ha. Proteins and RNAs display multilayer organization in nuclear speckles. (2017). (*co-corresponding authors; [§]equal contributors). *Journal of Cell Science*, **130**: 4180-4192.

24. T.S. Harmon, A.S. Holehouse, M.K. Rosen, **R.V. Pappu**. (2017). Intrinsically disordered linkers determine the interplay between phase separation and gelation in multivalent proteins. *eLife,* **6:**30294. **In the news:** https://source.wustl.edu/2017/12/engineers-uncover-design-principles-cellular-compartments/.

25. A. S. Holehouse, **R.V. Pappu**. (2017). FUS zigzags its way to cross beta. *Cell*, **171**: 499-500.

26. J. B. Warner IV[§], K. M. Ruff[§], 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). ([§]Co-first authors, *Co-corresponding authors). *Journal of the American Chemical Society,* **139:** 14456 – 14469. **In the news:** https://cen.acs.org/articles/95/i39/Revised-view-Huntingtons-protein-misfolding.html; https://source.wustl.edu/2017/10/imaging-a-killer/;

27. 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,* **114:** E9243 – E9252. **Selected and evaluated by Faculty of 1000.**

28. G. Fuertes[#], N. Banterle[#], K.M. Ruff[#], 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***, D. I. Svergun*, E. A. Lemke* ([#]Co-first authors, *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.

29. 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). **In the news:** https://www.eurekalert.org/pub_releases/2017-06/wuso-ncf062717.php.

30. M-T. Wei[#], S. Elbaum-Garfinkle[#], A.S. Holehouse[#], C. C-H. Chen, M. Feric, C.B. Arnold, R. D. Priestly, **R.V. Pappu***, C.P. Brangwynne*. (2017). Phase separation of intrinsically disordered proteins yields permeable, low-density liquid droplets. *Nature Chemistry*, **9:** 1118 – 1125. ([#]Co-first authors, *Co-corresponding authors). **In the news:** https://www.eurekalert.org/pub_releases/2017-06/wuis-dd062617.php; https://www.princeton.edu/news/2017/07/05/liquid-scaffolding-watery-droplets-form-structures-inside-cells.

31. J. Clarke, **R.V. Pappu**. Protein folding and binding, complexity comes of age. (2017). *Current Opinion in Structural Biology*, **42:** 5-7.

32. 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.

33. T.S. Harmon, A.S. Holehouse, **R.V. Pappu**. (2017). To mix, or to demix, that is the question. *Biophysical Journal*, **112**: 565-567, Invited New & Notable piece.
34. 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.
35. A. S. Holehouse*, R.K. Das, J. Ahad, M. O. G. Richardson, **R.V. Pappu***. (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.**
36. E.W. Martin†, A.S. Holehouse†, C.R. Grace, A. Hughes, **R.V. Pappu***, T. Mittag*. (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. (†Co-first authors; *Co-corresponding authors).
37. 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*, **29**: 339-346. **Selected and evaluated by Faculty of 1000.**
38. 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.
39. 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 subcompartments. *Cell*. **165:** 1-12. **In the news:** https://www.princeton.edu/news/2016/05/19/liquid-order-fluid-self-organizes-structure-controls-cell-growth-and-health.
40. R.K. Das, Y. Huang, A. Phillips, R.W. Kriwacki, **R.V. Pappu**. (2016). Cryptic sequence features within the disordered protein p27^{Kip1} regulate cell cycle signaling. *Proceedings of the National Academy of Sciences USA*. **113:** 5616-5621. **In the news:** https://phys.org/news/2016-05-cancer-cells-tracks.html.
41. 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.
42. 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.
43. C.P. Brangwynne, P.S. Tompa, **R.V. Pappu**. (2015). Polymer Physics of Intracellular Phase Transitions. *Nature Physics*. **11**: 899-904.
44. A.S. Holehouse, **R.V. Pappu**. Encoding phase transitions. (2015). *Nature Materials*. **14**: 1083-1084. Invited News & Views piece.
45. 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.
46. 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.

47. 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.

48. **R.V. Pappu** (2015). Cell signaling, division, and organization mediated by intrinsically disordered proteins. *Seminars in Cell and Developmental Biology.* **37**: 1-2.

49. 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.

50. 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.

51. 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.**

52. 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.

53. 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.**

54. **R.V. Pappu**. (2014). Frozen In Beta. *Biophysical Journal*. **107:** 795-797. Invited New & Notable Piece.

55. 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.**

56. 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.

57. 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).

58. 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.

59. 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.

60. 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.

61. 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.

62. 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.

63. A.K. Dunker et al. (2013). What's in a name? Why these proteins are called intrinsically disordered? *Intrinsically Disordered Proteins*. **1**: e24157.

64. N. Lyle, R.K. Das, **R.V. Pappu**. (2013). A quantitative measure for protein disorder. *The Journal of Chemical Physics*. **139**: 121907. PMID: 24089719.

65. 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.

66. 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.

67. 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.

68. 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*)

69. M.M. Babu, R.W. Kriwacki, **R.V. Pappu**. (2012). Versatility from protein disorder. *Science*, **337**: 1460-1461. PMID: 22997313.

70. 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.

71. 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.

72. R.K. Das, A.H. Mao, **R.V. Pappu**. (2012). Unmasking functional motifs within disordered regions of proteins. *Science Signaling*, **5**: pe17. PMID: 22510467.

73. 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.

74. 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.

75. 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.

76. 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.

77. 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.

78. D.G. Thomas, **R.V. Pappu**, Baker, NA. (2011). NanoParticle ontology for cancer nanotechnology research. *Journal of Biomedical Informatics*. **44**: 59-74. PMID: 20211274.

79. 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.

80. 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.

81. 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.

82. 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.

83. 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.

84. A.A. Chen, M. Marucho, N.A. Baker, **R.V. Pappu**. (2009). Simulations of RNA interactions with monovalent ions. *Methods in Enzymology*, **469**: 406-426. PMID: 2094680.

85. A. Vitalis, **R.V. Pappu**. (2009). Methods for Monte Carlo simulations of biomacromolecules. *Annual Reports in Computational Chemistry*. **5**: 49-76. PMID: 2042847.

86. D.G. Thomas, **R.V. Pappu**, N.A. Baker. (2009). NPO: Ontology for Cancer Nanotechnology Research. *Nature Precedings.* EMBC 2009. Annual International Conference of the IEEE. http://dx.doi.org/10.1109/IEMBS.2009.5333941.

87. H.A. Lashuel, **R.V. Pappu**. (2009). Amyloids Go Genomic: Insights Regarding the Sequence Determinants of Prion Formation from Genome-Wide Studies. *ChemBioChem,* **10**: 1951-1954. PMID: 19598186.

88. A. Vitalis, N. Lyle, **R.V. Pappu**. (2009). Thermodynamics of beta sheet formation in polyglutamine. *Biophysical Journal*, **97**: 303-311. PMID: 19580768. *Feature Article.*

89. A.A. Chen, D.E. Draper, **R.V. Pappu**. (2009). Molecular simulation studies of monovalent counterion-mediated interactions in a model RNA kissing loop. *Journal of Molecular Biology*, **390**: 805-819. PMID: 19482035.

90. **R.V. Pappu**, R. Nussinov. (2009). Protein folding: Lessons learned and new frontiers. *Physical Biology* **6**: 010301-1. PMID: 19208944.

91. A. Vitalis, **R.V. Pappu**. (2009). ABSINTH: A new continuum solvation model for simulations of polypeptides in aqueous solutions. *Journal of Computational Chemistry*, 30: 673-700. PMID: 18506808. *Cover picture*.

92. A. Vitalis, X. Wang, **R.V. Pappu**. (2008). Atomistic simulations of the effects of polyglutamine chain length and solvent quality on conformational equilibria and spontaneous homodimerization. *Journal of Molecular Biology*, **384**: 279-297. PMID: 18824003.

93. H.T. Tran, A. Mao, **R.V. Pappu**. (2008). Role of backbone-solvent interactions in determining conformational equilibria of intrinsically disordered polypeptides. *Journal of the American Chemical Society*, **130**: 7380-7392. PMID: 18481860.

94. M. A. Wyczalkowski, **R.V. Pappu**. (2008). Satisfying the fluctuation theorem in free energy calculations with Hamiltonian Replica Exchange. *Physical Review E*, **77**: 026104. PMID: 18352087.

95. **R.V. Pappu**, X. Wang, A. Vitalis, S.L. Crick. (2008). A polymer physics perspective on driving forces and mechanisms for protein aggregation. *Archives of Biochemistry and Biophysics*, **469**: 132-141. PMID: 17931593.

96. A.A. Chen, **R.V. Pappu**. (2007). Parameters of monovalent ions in the AMBER-99 forcefield: Assessment of inaccuracies and proposed improvements. *Journal of Physical Chemistry B*, **111**: 11884-11887. PMID: 17887792.

97. A. Vitalis, X. Wang, **R.V. Pappu**. (2007). Quantitative characterization of intrinsic disorder in polyglutamine: Insights from analysis based on polymer theories. *Biophysical Journal*, **93**: 1923-1937. PMID: 17526581.

98. A.A. Chen, **R.V. Pappu**. (2007). Quantitative characterization of ion pairing and cluster formation in strong 1:1 electrolytes. *Journal of Physical Chemistry B*, **111**: 6469-6478. PMID: 17526581.

99. S.L. Crick, M. Jayaraman, C. Frieden, R. Wetzel, **R.V. Pappu**. (2006). Fluorescence correlation spectroscopy shows that monomeric polyglutamine molecules form collapsed structures in aqueous solutions. *Proceedings of the National Academy of Sciences USA*, **103**: 1674-1679. PMID: 17075061.

100. H.T. Tran, **R.V. Pappu**. (2006). Toward an accurate theoretical framework for describing ensembles for proteins under strongly denaturing conditions. *Biophysical Journal*, **91**: 1868-1886. PMID: 16766618.

101. X. Wang, A. Vitalis, M.A. Wyczalkowski, **R.V. Pappu**. (2006). Characterizing the conformational ensemble of monomeric polyglutamine. *Proteins: Structure, Function and Bioinformatics*, **63**: 297-311. PMID: 16299774.

102. H.T. Tran, X. Wang, **R.V. Pappu**. (2005). Reconciling observations of sequence-specific conformational preferences with the generic behavior of denatured proteins. *Biochemistry*, **44**: 11369-11380. PMID: 16114874.

103. A. Patriciu, G.S. Chirikjian, **R.V. Pappu**. (2004). Analysis of the conformational dependence of mass-metric tensor determinants in serial polymers with constraints. *Journal*

of Chemical Physics, **121**: 12708-12720.

104. A.N. Drozdov, A. Grossfield, **R.V. Pappu**. (2004). The role of solvent in determining conformational preferences of alanine dipeptide in water. *Journal of the American Chemical Society*, **126**: 2574-2581. PMID: 14982467.

105. **R.V. Pappu**, G.D. Rose. (2002). A simple model for polyproline II structure in unfolded states of alanine-based peptides. *Protein Science*, **11**: 2437-2455.

106. **R.V. Pappu**, R. Srinivasan, G.D. Rose. (2000). The Flory isolated pair hypothesis is not valid for polypeptide chains: Implications for protein folding. *Proceedings of the National Academy of Sciences USA*, **97**: 12565-12570.

107. R.K. Hart, **R.V. Pappu**, J.W. Ponder. (2000). Exploring the similarities between potential smoothing and simulated annealing. *Journal of Computational Chemistry*, **97**: 12565-12570.

108. **R.V. Pappu**. Review of the Fourth Johns Hopkins Protein Folding Meeting. (1999). *Proteins: Structure Function, and Genetics*, **36**: 263-269.

109. **R.V. Pappu**, G.R. Marshall, J.W. Ponder. (1999). A potential smoothing algorithm accurately predicts transmembrane helix packing. *Nature Structural Biology*, **6**: 50-55.

110. **R.V. Pappu**, R.K. Hart, J.W. Ponder. (1998). Analysis and application of potential energy smoothing and search methods for global optimization. *Journal of Physical Chemistry B*, **102**: 9725-9742.

111. E.S. Huang, P. Koehl, M. Levitt, **R.V. Pappu**, J.W. Ponder. (1998). Accuracy of side-chain prediction upon near-native protein backbones generated by *ab initio* folding Methods. *Proteins: Structure, Function, and Genetics*, **33**: 204-217.

112. **R.V. Pappu**, D.L. Weaver. The early folding kinetics of apomyoglobin. (1998). *Protein Science*, **7**: 480-9742

113. **R.V. Pappu**, W.J. Schneller, D.L. Weaver. (1996). Electrostatic multipole representation of a polypeptide chain: An algorithm for simulation of polypeptide properties. *Journal of Computational Chemistry*, **17**: 1033-1045.

Submitted Manuscripts

1. L-P Bergeron-Sandoval, H. Khadivi Heris, C. Chang, C. E. Cornell, S. L. Keller, P. François, A. G. Hendricks, A. J. Ehrlicher, **R. V. Pappu***, S. W. Michnick*. A protein condensate drives actin-independent endocytosis. *Cell, revised version under review.* (*Co-corresponding authors)

2. I. Peran*, A.S. Holehouse*, I.S. Caricco, **R.V. Pappu**†, O. Bilsel†, D.P. Raleigh. Unfolded states under folding conditions accommodate sequence-specific conformational preferences alongside ensemble-averaged features of random coils. *Proceedings of the National Academy of Sciences USA, revised version under review* (*Co-first authors, †Co-corresponding authors).

3. 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. Cell*, *revised version under review*.

4. J. Guillén-Boixet, A. Kopach, J. Wang, A. S. Holehouse, D. Mateju, I. Poser, S. Maharana, M. Jahnel, M. Ruer-Gruß, D. Richter, D. Kuster, A. Honigmann, **R.V. Pappu**, A. A. Hyman, S. Alberti, T. M. Franzmann. A phosphorylation-controlled conformational switch drives stress granule formation by unlocking RNA multivalency. *Cell, under review.*

5. W. Bai, C. Sargent, J-M. Choi, **R.V. Pappu**, F. Zhang. Cyclized unimolecular protein nanostructures with ultra-high stability. *Nature Communications, revised version being prepared for submission following first round of reviews.*
6. E.W. Martin[†], I. Peran[†], A. S. Holehouse[†], M. Farag, J.J. Incicco, A. Bremer, C.R. Grace, A. Soranno, **R.V. Pappu**[§], T. Mittag[§] ([†]Co-first authors and [§]co-corresponding authors). Linking sequence-ensemble relationships and phase separation of a low complexity domain. *Submitted to Science.*

Manuscripts in preparation

1. J-M. Choi[†], F. Dar[†], **R.V. Pappu**. LASSI: A lattice-based bond-fluctuation model for system-specific simulations of phase transitions of multivalent proteins. *To be submitted to PLoS Computational Biology.* ([†]Co-first authors)
2. J-M. Choi, A.A. Hyman, **R.V. Pappu**. Interplay between two- and three-body interactions as drivers of percolation transitions in associative biopolymers. *In preparation for Physical Review Letters*.
3. D. Mitrea[†], J-M. Choi[†], C.B. Stanley, **R.V. Pappu[§]**, R.W. Kriwacki[§]. Structure of liquid-state condensates formed by multivalent proteins. *In preparation for Nature Structural Molecular Biology.* ([†]Co-first authors; [§]Co-corresponding authors)
4. J-M. Choi, D. Mitrea, R.W. Kriwacki, **R.V. Pappu**. Adaptation of the theory of molecular fluids for describing structures and dynamics of biomolecular condensates.
5. J-M. Choi, M.C. Cohan, F. Dar, A.S. Holehouse, A.E. Posey, K.M. Ruff, **R.V. Pappu**. Physical principles underlying the complex biology of intracellular phase transitions. *To be submitted as an invited contribution the Annual Review of Biophysics.*
6. M.C. Cohan, A.E. Posey, K.M. Ruff, A. Mittal, A.M.P. Eddelbuettel, S. J. Grigsby, P. A. Levin, **R.V. Pappu**. Patterning of oppositely charged residues within the intrinsically disordered tail of FtsZ modulates *in vitro* assembly and cell division in *B. subtilis. In preparation for Journal of Molecular Biology.*
7. M.C. Cohan, K.M. Ruff, A.S. Holehouse, **R.V. Pappu**. Evolutionary relationships inferred using quantitative measures for sequence-ensemble relationships of intrinsically disordered proteins.
8. M.C. Cohan, A.M.P. Eddelbuettel, K.M. Ruff, **R.V. Pappu**. A measured activity and assembly phase diagram for FtsZ.
9. F. Dar, J-M. Choi, **R.V. Pappu**. Mesoscale structures formed by phase transitions of linear multivalent proteins inferred from lattice simulations. *In preparation for Biophysical Journal.*
10. F. Dar, M.K. Rosen, **R.V. Pappu**. Comparative phase behavior of linear versus branched multivalent proteins comprising of folded domains and disordered regions.
11. F. Dar, J-M. Choi, **R.V. Pappu**. A general framework for closed-loop topologies of coexistence curves for the phase behavior of multi-component systems comprising of multivalent proteins.
12. M. J. Fossat, **R.V. Pappu**. *q*-canonical Monte Carlo: A novel method for modeling the impact of charge regulation on conformational distributions of disordered peptides. *In preparation for the Journal of Physical Chemistry B.*
13. M. J. Fossat, J-M. Choi, **R.V. Pappu**. Methods for multiscale simulations of intrinsically disordered proteins. *Invited review in preparation for Quarterly Reviews in Biophysics.*

14. M. J. Fossat, A.E. Posey, **R.V. Pappu**. *q*-Canonical Monte Carlo simulations help explain the formation of single alpha helices by sequences with patterned clusters of oppositely charged residues. *In preparation for the Journal of the American Chemical Society.*
15. G. Ginnel, M.C. Cohan, J. Lalmansingh, **R.V. Pappu**, A.S. Holehouse[†]. Sequence-based fingerprinting of intrinsically disordered proteins. *In preparation for Biophysical Journal.* ([†]Corresponding author)
16. A.S. Holehouse[†], J.M. Lalmansingh, K.M. Ruff, M.C. Cohan, **R.V. Pappu[†].** CTraj: A general-purpose analysis library for analyzing atomistic simulations of intrinsically disordered proteins. ([†]Co-corresponding authors). *In preparation for eLife.*
17. A.S. Holehouse, G. Ginnel, **R.V. Pappu.** An analytical framework for generating sequence-specific conformational distributions for proteins modeled as Flory random coils. *In preparation for Biophysical Journal.*
18. A.S. Holehouse, E.W. Martin, A.A. Hyman, T. Mittag, **R.V. Pappu**. Stickers and spacers formalism for the phase separation of prion-like domains. *In preparation.*
19. A.S. Holehouse[†], **R.V. Pappu**[†]. PIMMS: A coarse-grained simulation engine for deriving sequence-encoded phase diagrams of intrinsically disordered proteins from large-scale simulations of phase separation. ([†]Co-corresponding authors).
20. A.S. Holehouse, K.M. Ruff, **R.V. Pappu**. Sequence-specific emulsification in spontaneous formation of condensates.
21. A.S. Holehouse[§], **R.V. Pappu**[§]. Temperature sweep Metropolis Monte Carlo: A generalizable approach for enhanced sampling on rugged energy landscapes. *To be submitted to Journal of Chemical Physics*. ([§]Co-corresponding authors).
22. J. Lalmansingh, J.M. Choi[†], **R.V. Pappu**[†]. Mapping of free energy basin landscapes enables comparisons of residue-specific intrinsic conformational preferences. ([†]Co-corresponding authors).
23. J. Lalmansingh, K.M. Ruff, A.S. Holehouse, M.C. Cohan, **R.V. Pappu**. Parallelized algorithms for efficient reweighting of computationally derived ensembles for disordered proteins.
24. A.E. Posey[†], **R.V. Pappu**[†]. Experimental methods and theoretical analysis for mapping coexistence curves of biological macromolecules. ([†]Co-corresponding authors).
25. A.E. Posey[†], T.S. Harmon, M. J. Fossat, **R.V. Pappu**[†]. Preferential neutralization of ionizable residues stabilizes alpha helices in sequences with patterned clusters of oppositely charged residues. *In preparation for the Journal of the American Chemical Society.* ([†]Co-Corresponding authors).
26. K.M. Ruff[†], **R.V. Pappu**[†]. Assessment of theoretical versus computational approaches for predicting the dimensions of intrinsically disordered proteins. ([†]Co-corresponding authors).
27. K. M. Ruff, A.E. Posey, **R.V. Pappu.** Polyphasic Linkage: A thermodynamic framework for understanding how ligand binding influences phase separation. *In preparation.*
28. K.M. Ruff, A.E. Posey, **R.V. Pappu**. Generalization of the polyphasic linkage formalism to model the impacts of networks of ligands on protein phase behavior. *In preparation for Biophysical Journal.*
29. K.M. Ruff[†], M.O.G. Richardson, A.S. Holehouse, **R.V. Pappu**[†]. Evolutionary analysis of polar tracts and their sequence contexts across proteomes. ([†]Co-corresponding authors).

30. K.M. Ruff[†], M.C. Cohan[†], **R.V. Pappu**. Multiscale computational analysis of the impact of disordered tails on FtsZ conformations and assembly. ([†]Co-first authors)
31. X. Zeng, J-M. Choi, A. Chilkoti, **R.V. Pappu.** High-throughput computational design of intrinsically disordered protein polymers that undergo thermo-responsive phase behavior.
32. X. Zeng[†], K.M. Ruff[†], **R.V. Pappu**. Enhancing machine learning aided coarse-grained simulations of intrinsically disordered protein polymers using cycles of active learning and refinement. *In preparation for the Journal of Physical Chemistry B.* ([†]Co-first authors)
33. X. Zeng, J-M. Choi, A.S. Holehouse, A. Chilkoti, **R.V. Pappu**. A multiscale pipeline for predicting phase diagrams of individual chains and collections of thermo-responsive intrinsically disordered protein polymers.
34. T.S. Harmon, S. Roberts, A. Chilkoti, **R.V. Pappu**. A physical model for programmable hysteresis in partially ordered protein polymers that undergo thermoresponsive phase transitions.

Grants

CURRENT

National Science Foundation, DMR 1729783 – 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), RGP0034/2017
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 – December 31, 2020
Principal Investigators: Rohit Pappu (contact PI), Marc I. Diamond, and Ralf Langen

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

PENDING

National Institutes of Health, 1R01NS105497
Title: *Huntingtin conformation and neurodegeneration*
Principal Investigators: Steven Finkbeiner (contact PI)**, Rohit Pappu (co-PI)**
Role in the project: *Principal Investigator* in Multi-PI grant

National Institutes of Health, 1R01 GM131148
Title: *Sequence Determinants of the conformations and functions of disordered proteins that undergo multisite phosphorylation*
Principal Investigators: Tanja Mittag (contact PI), Rohit Pappu (co-PI)
Co-Investigators: Barak Cohen, Benjamin Schuler
Role in the project: *Principal Investigator* in Multi-PI grant

COMPLETED

National Institutes of Health, 1RO1GM108785
Title: *Signal transduction by ERBB2 / ERBB3 oligomers*
Funding period: October 01, 2013 – March 31, 2017
Principal Investigator: Linda J. Pike
Role in the project: *Co-Investigator*

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 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.

RESEARCH MENTORING

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

1. **Jeong-Mo Choi,** Postdoctoral Scientist
2. **Martin Fossat,** Postdoctoral Scientist
3. **Alex S. Holehouse,** Postdoctoral Scientist
4. **Ammon E. Posey,** Research Scientist
5. **Kiersten M. Ruff,** Postdoctoral Scientist
6. **Max V. Staller,** Co-mentored Postdoctoral Scientist (primary mentor: Barak A. Cohen)
7. **Xiangze Zeng,** Postdoctoral Scientist

***Current Doctoral Students* (*alphabetical order*)**

1. **Megan C. Cohan**, Doctoral Student, Department of Biomedical Engineering. Projected graduation date, May 2020.
2. **Furqan Dar,** Doctoral Student, Department of Physics, Projected graduation date, December 2021.
3. **Jared M. Lalmansingh**, Doctoral Student, Department of Physics. Projected graduation date, December 2020.
4. **Andrew Z. Lin**, Doctoral Student, Division of Biology & Biomedical Sciences, Program Plant and Microbiology. Projected graduation date, August 2021.

***Current Undergraduate Students* (*alphabetical order*)**

1. **Anna M. P. Eddelbuettel**, Third-year student in the Department of Biomedical Engineering. Scheduled to graduate, May 2020.

***Current Research Staff* (*alphabetical order*)**

1. **Garrett Ginell**, Junior Computational Research Scientist, August 2019 onward.
2. **Catherine Kornacki,** Laboratory Research Technician, August 2019 onward.

Lab alumni – reverse chronological order

1. **Mary O. G. Richardson,** Junior Research Scientist and Scientific Programmer, August 2017 – June 2018.
2. **Sang Eun Jee**, Postdoctoral Scientist, November 2016 – October 2017.
3. **Kourtney L. Kroll,** Undergraduate researcher, Summer 2017.
4. **Divya Natarajan,** MD Student, Washington University School of Medicine, graduation date, May 2020.
5. **Tyler S. Harmon**, Doctoral Student, Department of Physics. Received PhD in April 2017. Currently, postdoctoral scientist at the Max Planck Institute in Dresden, Germany.
6. **Rajni Verma**, Postdoctoral Scientist, October 2015 – June 2016.
7. **Rahul K. Das**, Postdoctoral Scientist. Currently, a senior research scientist at GNS Healthcare, Cambridge, MA.
8. **Anuradha Mittal**, Postdoctoral Scientist. Currently, a senior Bioinformatics Scientist at Affymetrix, San Francisco, CA.
9. **Laruen M. Bedell**, Undergraduate Student, Department of Biomedical Engineering.
10. **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.
11. **James Ahad**, Undergraduate student, Biomedical Engineering. Currently, an MSTP student at Case Western University School of Medicine.
12. **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.

13. **Siddique J. Khan**, Postdoc, April 2012 – May 2013.
14. **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.
15. **Tony Wang**, Summer undergraduate researcher, Summer 2012.
16. **Marta Wells**, Summer undergraduate research, Summer 2011 and 2012. Currently a graduate student in Computational Biology at Carnegie-Mellon University.
17. **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.
18. **Jordan Nick**, Summer HHMI undergraduate fellow, Summer 2011.
19. **Kelly Culhane**, SURF student, Summer 2011. Currently, a Ph.D. student in Biochemistry & Biophysics at Yale University.
20. **Aditya Radhakrishnan**, Master's student (BS/MS), Summer 2010 – Summer 2011. Currently Ph.D. student in Computational & Molecular Biophysics at Johns Hopkins University.
21. **Nil Gural,** Undergraduate researcher, Spring 2011. Currently Ph.D. student in the Harvard-MIT Health Sciences Program.
22. **Adam T. Steffen**, Scientific programmer, Summer 2007 – December 2010. Currently a software engineer at Partek Inc., Chesterfield, MO.
23. **Alexander French**, Undergraduate researcher, Summer 2010. Currently graduate student in Biochemistry & Biophysics at the University of Chicago.
24. **Anil Kumar**, Postdoctoral scientist, December 2009 – August 2010. Currently a postdoc at the University of Toronto in synthetic organic chemistry.
25. **Caitlin L. Chicoine**, Undergraduate researcher, Summer of 2009, Graduated from Washington University, School of Engineering & Applied Sciences Valedictorian.
26. **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.
27. **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.
28. **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.
29. **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.
30. **Jose Pulido**, Undergraduate Trainee, May 2008 – October 2008.

31. **Xiaoling Wang**, Research scientist, September 2004 – February 2008. Currently a staff scientist at Pfizer Inc. in St. Louis, MO.
32. **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.
33. **Alexander N. Drozdov**, Postdoctoral Scientist, September 2002 – April 2004. Currently at Mentor Graphics, San Jose, CA; Senior scientist in the photolithography research group.
34. **Magdalena Fus**, Undergraduate Trainee, September 2004 – May 2005.
35. **Tirath Patel**, Undergraduate Trainee, September 2004 – May 2005.

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

1. Princeton University, Department of Chemical & Biochemical Engineering, May 2018
2. University of California, Berkeley, Molecular and Cell Biology, April 2017
3. Hospital for Sick Kids, Toronto, Molecular Medicine Seminar Series, March 2017
4. Washington University, Department of Genetics Seminar Series, February 2017
5. McGill University, Department of Biology, January 2017
6. Princeton University, Department of Chemical & Biochemical Engineering, December 2016
7. Tata Institute for Fundamental Research, Mumbai, India, November 2016
8. Department of Biomedical Engineering, Washington University in St. Louis, October 2016
9. MRC Laboratory of Molecular Biology, Cambridge, UK, June 2016
10. Johns Hopkins University, Department of Materials Science, April 2016
11. Hiroshima University, December 2015
12. Duke University, NSF-MRSEC, April 2015
13. University of British Columbia, Center for High-Throughput Biology, April 2015
14. Washington University in St. Louis, Biophysical Evening, January 2015
15. University of Texas Southwestern Medical Center, Department of Biophysics, December 2014
16. University of Cambridge, Department of Chemistry, November 2014
17. MRC Laboratory of Molecular Biology, Cambridge, UK, November 2014
18. Stony Brook University, Laufer Center for Quantitative Biology, November 2014
19. Kansas State University, Department of Biochemistry, April 2014
20. Ohio State University, Department of Biochemistry, Biophysics Program, April 2014
21. University of Montana, Department of Chemistry & Biochemistry, February 2014
22. Johns Hopkins University, Department of Biophysics, December 2013
23. University of Wisconsin-Madison, Department of Chemical & Biochemical Engineering, December 2013
24. University of Zurich, Department of Biochemistry, September 2013
25. The Scripps Research Institute, Department of Molecular & Experimental Medicine, July 2013
26. University of Texas Southwestern Medical Center, University Colloquium, July 2013

27. University of Texas Southwestern Medical Center, Green Center for Systems Biology, Special Seminar, July 2013
28. Symposium on Physics and Biology of Strongly Fluctuating Proteins, University of Maryland, May 2013
29. American Chemical Society Meeting, New Orleans, April 2013
30. University of Chicago, Institute for Biophysical Dynamics, April 2013
31. March Meeting of the American Physical Society, Baltimore, March 2013
32. CUNY City College of New York, Structural Biology Colloquium, March 2013
33. 57th Annual Meeting of the Biophysical Society, Philadelphia, Protein Electrostatics Symposium
34. University of Minnesota, Department of Biomedical Engineering, December 2012
35. Protein Folding Consortium, PIs meeting, Chicago, November 2012
36. International Symposium on Protein Folding, National Centre for Biological Sciences, Bangalore, India, October 2012
37. Protein Folding Consortium, SUNY Stony Brook, NY, June 2012
38. Biopolymers Gordon Research Conference, Newport, RI, June 2012
39. Hope Center for Neurological Disorders, Washington University, May 2012
40. Arizona State University, Center for Biological Physics, Tempe, AZ, April 2012
41. University of South Florida, Department of Physics, Tampa, FL, March 2012
42. St. Jude Children's Research Hospital, Memphis, TN, January 2012
43. CCP 2011 – Conference on Computational Physics, Knoxville, TN, November 2011
44. National Science Foundation Workshop on Future of RNA and Protein Folding, Arlington, VA, September 2011
45. University of Leeds, UK, July 2011
46. MRC Laboratory of Molecular Biology, Cambridge, UK, July 2011
47. Annual Meeting of the Protein Folding Consortium, UC Berkeley, June 2011
48. University of Texas Southwestern Medical School, May 2011
49. The Scripps Research Institute, Molecular & Experimental Medicine, May 2011
50. Washington University School of Medicine, Computational & Molecular Biophysics Program, Biophysical Evening Series, May 2011
51. Midwest Conference on Protein Folding, Assembly, and Molecular Motions, May 2011
52. 55th Annual Meeting of the Biophysical Society, Baltimore, MD, March 2011
53. Department of Biochemistry, Cornell Weill Medical College, December 2010
54. ACS Midwest Regional Meeting Symposium on Protein Folding, October, 2010
55. Intrinsically disordered proteins, Keynote Session Chair, Gordon Research Conference, North Carolina, July 2010.
56. Protein folding pathways workshop, Arizona State University, May 2010.
57. University of Pittsburgh School of Medicine, March 2010.
58. Yale University, Biophysics program, January 2010.
59. Protein folding and dynamics, Gordon Research Conference, January 2010.
60. The Scripps Research Institute, Molecular & Experimental Medicine, November 2009.
61. 23rd Annual Gibbs conference on Biothermodynamics, Carbondale, IL, October 2009.
62. Tata Institute of Fundamental Research, Mumbai, India, August 2009.
63. Argonne National Laboratory, Biology Division, August 2009.
64. Northwestern University, Biochemistry, Molecular Biology & Cell Biology, July 2009.

65. Telluride Scientific Research Conference, Workshop on RNA dynamics, July 2009.
66. FASEB Amyloid meeting, Snowmass, CO, June-July 2009.
67. University of California Berkeley, Department of Bioengineering, April 2009.
68. MIT-Whitehead Institute, Department of Biology, March 2009.
69. Annual Meeting of the Biophysical Society, Invited Workshop, Boston, MA, March 2009.
70. Department of Chemistry & Biochemistry, University of Massachusetts, Amherst, MA, February 2009
71. Rice University, Department of Chemistry, November 2009.
72. Rensselaer Polytechnic Institute, Biocomputation seminar series, October 2008.
73. 22nd Annual Symposium of the Protein Society, July 2008, San Diego, CA
74. Protein Electrostatics Workshop, Telluride, CO, July 2008
75. Biopolymers Gordon Research Conference, Newport, RI, June 2008.
76. University of Texas Austin, Department of Biomedical Engineering, April 2008.
77. University of Oregon, Department of Chemistry, April 2008.
78. Intrinsically Disordered Proteins subgroup meeting, Annual meeting of the Biophysical Society, Long Beach, CA, February 2008
79. The Scripps Research Institute, Department of Chemistry, La Jolla, CA, September 2007.
80. Gordon Research Conference: Proteins, June 2007, Holderness, New Hampshire.
81. Washington University in St. Louis, Biophysical Evening Series, December 2007.
82. University of California in Santa Barbara, Department of Chemistry, April 2007.
83. University of Delaware, Department of Chemistry and Biochemistry, April 2007.
84. Indiana University, Computational Biology and Bioinformatics, September 2006.
85. National Cancer Institute, Frederick, August 2006.
86. FASEB Amyloid Meeting, Snowmass, Colorado, June 2006.
87. DIMACS Workshop on Computational / Experimental Approaches to Protein Defects in Human Disease, Rutgers University, April 2006.
88. University of North Carolina, Chapel Hill, Department of Chemistry, April 2006.
89. Duke University, Department of Biochemistry, April 2006.
90. UTMB, Galveston, TX, Sealy Center for Structural Biology, April 2006.
91. Johns Hopkins University, Department of Chemistry, March 2006.
92. Stanford University, Department of Chemistry, March 2006.
93. I2CAM Exploratory Workshop on Protein Aggregation and Amyloid Formation in Systemic and Neurodegenerative Diseases: Physical, Molecular, and Biological Approaches, EPFL, Lausanne, Switzerland, July 2005.
94. 18th Annual Gibbs Conference on Biothermodynamics, Carbondale IL, October 2004.
95. University of Iowa, Department of Chemistry, Iowa City, May 2004.
96. Washington University, Alzheimer's disease Research Center, April 2004.
97. Washington University, Department of Genetics, October 2002.
98. Washington University, Alzheimer's disease Research Center, December 2002.
99. 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 co-chaired the strategic planning committee commissioned by the Dean of the School of Engineering & Applied Sciences. The goal was 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 *Biochemical Journal*, *Biochemistry*, *Biomacromolecules, Biophysical Journal, Biophysical Chemistry, Cell, Cell Reports, eLife, 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, 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.