

ROHIT V. PAPPU

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PROFESSIONAL BACKGROUND

Academic Positions

September 2021 – current: Gene K. Beare Distinguished Professor of Engineering, McKelvey School of Engineering, Washington University in St. Louis

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

March 2015 – August 2021: Edwin H. Murty Professor of Engineering, McKelvey School of Engineering, Washington University in St. Louis

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

Professional Societies

Member, American Association for the Advancement of Science (AAAS)

Member, American Chemical Society (ACS)

Member, American Institute of Medical and Biological Engineers (AIMBE)

Member, Biophysical Society (BPS) and subgroups on Intrinsically Disordered Proteins (IDPs) and Biopolymers In Vivo (BIV)

Member, The Protein Society (TPS)

Member, Sigma Xi, The Scientific Honor Society

ACTIVE RESEARCH PROGRAM

Cellular Organization Molecular Biophysics & Bioengineering

Our research is focused on uncovering the biophysical principles underlying the spatial and temporal organization of cellular matter, its impact on cell physiology and disease, and leveraging fundamental insights for designing novel materials and biomolecular condensates. Our investigations span multiple length scales and involve a collective effort on the biophysical principles pertaining to the form, function, regulation, phase behavior, and evolution of intrinsically disordered and multivalent proteins. Our research directly impacts topics of biomedical relevance that include the molecular basis of neurodegeneration, phase transitions that lead to protein and RNA condensates, the biophysics of molecular recognition via soft and disordered interfaces, and the design of responsive, protein-based biomaterials. Our work is driven by a blend of novel multiscale computer simulations, adaptations and developments of polymer physics theories, the physics of active matter and non-equilibrium statistical physics of living systems. We close the loop with *in vitro* and in cell experiments performed in my lab and through a vibrant network of international collaborations.

Intrinsically disordered proteins (IDPs): Between 30% and 50% of eukaryotic proteomes comprise of intrinsically disordered proteins / regions (IDPs / IDRs). Over the years, we have uncovered sequence-ensemble relationships of IDPs / IDRs that connect the information encoded in amino acid sequences to quantitative descriptions of conformational ensembles. These efforts have yielded predictive descriptions and uncovered the rich contributions made by amino acid composition, charge content, and sequence patterning effects to the global sizes, shapes, amplitudes of conformational fluctuations, and context dependent secondary structural preferences within IDPs / IDRs. These discoveries have been made possible through novel combinations of polymer physics theories, accurate and efficient molecular simulations driven by our homegrown ABSINTH implicit solvation model, and biophysical experiments. In ongoing investigations, we are pursuing three new avenues: (1) We are using computationally driven approaches to design novel IDPs / IDRs with bespoke sequence-ensemble relationships to uncover the connections between these relationships and molecular functions, especially in the context of transcriptional regulation. (2) We are developing and deploying new, multiscale computational and theoretical approaches to model circuits controlled by multisite phosphorylation and other multisite post-translational modifications within IDPs / IDRs. (3) We are deploying new methods to investigate the effects of sequence-specific charge regulation, specifically proton uptake and release phenomena on disorder-order transitions of IDPs / IDRs in cellular milieus.

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 sol-gel transitions as well as liquid-liquid, liquid-solid, and liquid-liquid crystalline phase separation. Our focus is on describing relationships between protein sequences / architectures and the stimulus specific phase diagrams that are governed by spontaneous driving forces also known as passive processes. This focus is driven by the importance of biomolecular condensates that form via phase transitions afford spatiotemporal organization and information transduction within cells. Specific foci include nuclear bodies, stress responses, synaptic bodies, and the interplay between spontaneous and driven processes. We are also embarking on rigorous dynamical and structural descriptions of biomolecular condensates with a view to uncovering how driven (active) processes influence spatiotemporal regulation in living cells.

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.

Intrinsically disordered regulome in bacteria: Although IDPs / IDRs represent only 5% of typical bacterial proteomes, it has become clear that almost all key aspects that control bacterial life cycles are controlled by IDPs / IDRs. Often these sequences are hypervariable and the implications an emerging goal in my lab is to uncover how IDPs / IDRs influence functional outcomes in bacteria. These studies are being driven by multilevel theory, computation, biochemical experiments, and high-throughput library-based in vivo investigations. The long-term goal is to combine bottom-up and top-down investigations to make headway into the design of bacterial communities with bespoke emergent properties and the selective inhibition of bacteria by targeting IDPs / IDRs using novel antibiotics.

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

Awards

Inducted, by election, as a full member of the Sigma Xi Scientific Research Honor Society, January 2020

Recipient of the 2019 McKelvey Engineering Faculty Award for excellence in teaching, Washington University in St. Louis, April 2019

Named as Mercator Fellow by the Deutsche Forschungsgemeinschaft (DFG), May 2019 – April 2022

Elected Fellow of the Biophysical Society, 2019

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.

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

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

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

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

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

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

Honors

Member, Board of Reviewing Editors for eLife – January 2021 – present

Listed, in 2020, by the Institute of Science as being in the top 0.5% of researchers worldwide in terms of number of citations

Listed, in 2019, by the Institute of Science as being in the top 1% of researchers worldwide in terms of number of citations

Chair of NIH ZRG1-MDCN study section, April 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

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

Guest Editor, *Current Opinion in Structural Biology*, 2017

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

Member, Editorial Advisory Board, *Biophysical Journal*, December 01, 2014 – December 31, 2020

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

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

Named / Keynote Lectures and Webinars

Keynote talk, Preamble to the IDPSIG and IDP Seminars joint Early Career Scientists virtual poster session, September 2021.

Mercator Fellow Keynote Lecture, *DFG Priority Program on Phase Separation*, Virtual meet, real eat conference, March 2021.

Student invited seminar speaker, University of Halle, March 08, 2021

Student and postdoc invited speaker, student / postdoc retreat of the *DFG Priority Program on Phase Separation* (SPP2191), Heidelberg, Germany, May 2020 – postponed due to Covid-19.

Student Invited Colloquium Speaker, University of Washington, *Physical Chemistry Series*, Seattle, WA, February 2020.

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

Featured speaker, American Chemical Society Webinar Series, Phase Separation of Multivalent Proteins, co-produced with Biochemistry, November 2019

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

Student Invited Closing Keynote Speaker for Gordon Research Seminar on Computational Aspects of Biomolecular NMR, Les Diablerets, Switzerland, June 2019: *Uncovering the marvels of protein conformational heterogeneity along roads less traveled.*

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

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.

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

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

Opening Keynote 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.

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.

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

Invited Talks at National and International Conferences / Symposia / Workshops

Invited Speaker, Cell Symposia on *Biological Assemblies: Phase separation and more*, Seville, Spain, October 31 – November 03, 2021.

Invited Speaker, 2021 Online Meeting of the German Society of Cell Biology, *Life in between – The Cell Biology of Interfaces*, Plenary speaker in session on Phase Separation and Membraneless Organelles, Münster, Germany, September 2021.

Invited Speaker, *Genome Biology and Disease Meeting*, Organized by AAAS and Science Magazine, Virtual globally and in person in China, September 2021.

Invited Speaker, Telluride Science Research Conference on *Intrinsically Disordered Proteins*, July 2021.

Invited Speaker, *Protein Folding & Dynamics*, Webinar series, July 2021.

Invited Speaker, *FASEB meeting on Protein Aggregation*, Virtual meeting, June 2021.

Invited Speaker, Online meeting *Phase Separated Systems in the Nucleus (PSINU)*, hosted by IISER Pune, India, April 6 – 9, 2021

Invited Speaker, *Proteostasis consortium*, Weekly seminar series, March 10, 2021

Invited Speaker, 3rd RIKEN Biosystems Dynamics Research Symposium – *Structuring biosystems: functions emerging from molecules*. Virtual event, March 1-3, 2021.

Invited speaker, <http://condensates.com> kitchen table talk series. Delivered three separate one-hour lectures as part of a series focused on the Molecular Grammar of Biomolecular Condensate Formation and Regulation. July and August 2020.

Invited Speaker, NSF Sponsored Workshop and International Summer School on *Genome Architecture and Dynamics*, Massachusetts Institute of Technology, Cambridge, MA, June 2020 – postponed due to Covid19.

Invited Speaker, Canadian Institute for Advanced Research (CIFAR) symposium on *Scaling in Complexity to Living Systems – Molecular Architecture of Life*, Vancouver, Canada, April 2020 – canceled due to Covid-19.

Invited Speaker, 2020 *Symposium on Intrinsically Disordered Proteins: From fundamental biology to disease*, organized by the Intrinsically Disordered Proteins Specific Interest Group (IDPSIG), Stanford University, February 2020.

Invited Speaker, Telluride Science Research Conference on *Intrinsically Disordered Proteins*, Telluride, CO, July 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, *Session on Phase Separation*, 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.
- 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.

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

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

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

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

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

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

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

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

Invited Speaker, 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 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

Peer Reviewed Publications (reverse chronological order) includes articles in press (Google scholar h-index: 62; i10 index 118)

- Pub.01.** A. Bremer[§], M. Farag[§], W.M. Borchers[§], I. Peran, E.W. Martin, **R.V. Pappu**[†], T. Mittag[†]. (2021). Deciphering how naturally occurring sequence impact the phase behaviors of disordered prion-like domains. ([§]Co-first authors; [†]Co-corresponding authors). *Nature Chemistry*, in press.
- Pub.02.** K.M. Ruff, **R.V. Pappu**. (2021). AlphaFold and implications for intrinsically disordered proteins. *Invited, peer-reviewed perspective. Journal of Molecular Biology*, in press. <https://doi.org/10.1016/j.jmb.2021.167208>.
- Pub.03.** K.M. Ruff, F. Dar, **R.V. Pappu**. (2021). Polyphasic linkage and the impact of ligand binding on the regulation of biomolecular condensates. *Biophysics Reviews*, **2**: 021302.
- Pub.04.** M.J. Fossat[†], X. Zeng[†], **R.V. Pappu**. (2021) Uncovering differences in hydration free energies and structures for model compound mimics of charged sidechains of amino acids. ([†]Co-first authors). *Journal of Physical Chemistry B*, **125**: 4148-4161.
- Pub.05.** A.E. Posey^{§,†}, K.M. Ruff[§], J.M. Lalmansingh[§], T. Kandola, R. Halfmann, **R.V. Pappu**[†]. (2021). Mechanistic inferences from analysis of measurements of protein phase transitions in live cells. ([§]Co-first authors; [†]Co-corresponding authors). *Journal of Molecular Biology*, **433**: 166848.
- Pub.06.** X. Zeng, C. Liu, M.J. Fossat, P. Ren, A. Chilkoti, **R.V. Pappu**. (2021). Design of intrinsically disordered proteins that undergo phase transitions with lower critical solution temperatures. *APL Materials*, **9**: 021119.
- Pub.07.** K.M. Ruff^{§,†}, F. Dar[§], **R.V. Pappu**[†]. Ligand effects on phase separation of multivalent macromolecules. (2021). ([§]Co-first authors; [†]Co-corresponding authors). *Proceedings of the National Academy of Sciences USA*, **118**: e2017184118.
- Pub.08.** T. Lazar, E. Martínez-Pérez, F. Quaglia⁵, A. Hatos, L. B. Chemes, J.A. Iserte, N. A. Méndez, N. A. Garrone, T. E. Saldaño, J. Marchetti, A. J. Velez Rueda, P. Bernado, M. Blackledge, T. N. Cordeiro, E. Fagerberg, Julie D. Forman-Kay, M. S. Fornasari, T. J. Gibson, G-N. W. Gomes, C. C. Gradinaru, T. Head-Gordon, M. R. Jensen, E. A. Lemke, S. Longhi, C. Marino-Buslje, G. Minervini, T. Mittag, A. M. Monzon, **R.V. Pappu**, G. Parisi, S. Ricard-Blum, K. M. Ruff, E. Salladini, M. Skepö, D. Svergun, S. D. Vallet, M. Varadi, P. S. Tompa*, S. C.E. Tosatto*, D. Piovesan. (2021). PED in 2021: A major update of the protein ensemble database for intrinsically disordered proteins. *Nucleic Acids Research*, **49**: D404-D411.
- Pub.09.** M. Lorenzini, S. Burel, A. Lesage, E. Wagner, C. Charrière, P-M. Chevillard, M. Bérangère, D. Maloney, K.M. Ruff, **R. V. Pappu**, S. Wagner, J.M. Nerbonne, J. R. Silva, R.R. Townsend, L.S. Maier, C. Marrionneau. (2021). Proteomic and functional mapping of cardiac Na_v1.5 channel phosphorylation reveals multisite regulation of surface expression and gating. *Journal of General Physiology*, **153**: e202012646.
- Pub.10.** C. Mathieu, **R.V. Pappu**, J.P. Taylor. (2020). Beyond aggregation: pathological phase transitions in neurodegenerative disease. *Science*, **370**: 56-60.

- Pub.11.** J-M. Choi, A.A. Hyman, **R.V. Pappu**. (2020). Generalized models for bond percolation transitions of associative polymers. *Physical Review E*, **102**: 042403.
- Pub.12.** F. Dar, **R.V. Pappu**. (2020). Restricting the size of condensates. *eLife*, **9**:e59663. *Invited and reviewed insight article*.
- Pub.13.** X. Zeng, A.S. Holehouse, A. Chilkoti, T. Mittag, **R.V. Pappu**. (2020). Connecting coil-globule transitions to full phase diagrams for intrinsically disordered proteins. *Biophysical Journal*. **119**: 1- 17.
- Pub.14.** M.C. Cohan, **R.V. Pappu**. (2020). Making the case for disordered proteins and biomolecular condensates in bacteria. *Trends in Biochemical Sciences*, **45**: 668-680.
- Pub.15.** M.C. Cohan, A.M.P. Eddelbuettel, P.A. Levin, **R.V. Pappu**. Dissecting the functional contributions of the intrinsically disordered C-terminal tail of *B. subtilis* FtsZ. (2020). *Journal of Molecular Biology*, **432**: 3205 – 3221.
- Pub.16.** J. Guillén-Boixet, A. Kopach, A. S. Holehouse, S. Wittmann, M. Jahnel, R. Schlüßler, I. R. E. A. Trussina, J. Wang, D. Mateju, I. Poser, S. Maharana, M. Ruer-Gruß, D. Richter, Y-T. Chang, A. Honigmann, A. A. Hyman, **R.V. Pappu**, S. Alberti, T. M. Franzmann. (2020) RNA induces conformational rearrangements and clustering of G3BP that drive condensation and stress granule formation. *Cell*, **181**: 346-361.
- Pub.17.** J. A. Greig, T.A. Nguyen, M. Lee, A. S. Holehouse, A.E. Posey, **R.V. Pappu**, G.J. Jedd. Arginine-enriched mixed-charge domains provide cohesion for nuclear speckle condensates. (2020). *Molecular Cell*, **77**: 1-14.
- Pub.18.** E.W. Martin[†], A. S. Holehouse[†], I. Peran[†], M. Farag, J.J. Incicco, A. Bremer, C.R. Grace, A. Soranno, **R.V. Pappu**[§], T. Mittag[§]. (2020). ([†]Co-first authors and [§]co-corresponding authors). Valence and patterning of aromatic residues determine the phase behavior of prion-like domains. *Science*. **367**: 694-699.
- Pub.19.** J-M. Choi, A.S. Holehouse, **R.V. Pappu**. (2020). Physical principles underlying the complex biology of intracellular phase transitions. *Annual Review of Biophysics*, **49**: 107-133.
- Pub.20.** J-M. Choi[†], F. Dar[†], **R.V. Pappu**. (2019). LASSI: A lattice model for simulating phase transitions of multivalent proteins. ([†]Co-first authors). *PLoS Computational Biology*, **15**: e1007028.
- Pub.21.** M. J. Fossat, **R.V. Pappu**. (2019). *q*-Canonical Monte Carlo sampling for modeling the linkage between charge regulation and conformational equilibria of peptides. *Journal of Physical Chemistry B*, **123**: 6952-6967.
- Pub.22.** M.C. Cohan, K.M. Ruff, **R.V. Pappu**. (2019). Information theoretic measures for quantifying sequence-ensemble relationships of intrinsically disordered proteins. *Protein Engineering, Design, and Selection*, **32**: 191-202.
- Pub.23.** S.K. Powers, A.S. Holehouse, D.A. Korasick, K.H. Schreiber, E. Tycksen, J.M. Jez, **R.V. Pappu**, L.C. Strader. (2019). Nucleo-cytoplasmic partitioning of ARF proteins control auxin responses in *Arabidopsis thaliana*. *Molecular Cell*, **76**: 175-190.e5.
- Pub.24.** W. Bai, C. Sargent, J-M. Choi, **R.V. Pappu**, F. Zhang. (2019). Covalently assembled single chain protein nanostructures with ultrahigh stability. *Nature Communications*, **10**: 3317.
- Pub.25.** J. Cable, C. Brangwynne, G. Seydoux, D. Cowburn, **R.V. Pappu**, C.A. Castañeda, L.E. Berchowitz, Z. Chen, M. Jonikas, A. Dernburg, T. Mittag, N.L. Fawzi.

Phase separation in Biology and Disease – a symposium report. (2019). *Annals of the New York Academy of Sciences*. **1452**: 3-11.

- Pub.26.** I. Peran*, A.S. Holehouse*, I.S. Caricco, **R.V. Pappu**[†], O. Bilsel[†], D.P. Raleigh. (2019). 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*. **116** (25): 12301 – 12310. (*Co-first authors; [†]Co-corresponding authors).
- Pub.27.** 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*. **116** (16): 7889-7898. ([†]Co-corresponding authors).
- Pub.28.** 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. *Journal of the American Chemical Society*, **141**(12): 4908-4918. (*Co-first authors).
- Pub.29.** 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.
- Pub.30.** 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.
- Pub.31.** 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).
- Pub.32.** 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).
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- Pub.123.** **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.
- Pub.124.** **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.
- Pub.125.** 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.
- Pub.126.** **R.V. Pappu**, D.L. Weaver. The early folding kinetics of apomyoglobin. (1998). *Protein Science*, **7**: 480-9742
- Pub.127.** **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.

Commentaries, editorials, meeting reviews, and perspectives

- Com. 1.** R.V. Pappu. (2020). Phase separation – a physical mechanism for organizing information and biochemical reactions. *Developmental Cell*, **55**: 1-3.
- Com. 2.** 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.
- Com. 3.** 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.
- Com. 4.** A. S. Holehouse, R.V. Pappu. (2017). FUS zigzags its way to cross beta. *Cell*, **171**: 499-500.
- Com. 5.** 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.
- Com. 6.** J. Clarke, R.V. Pappu. Protein folding and binding, complexity comes of age. (2017). *Current Opinion in Structural Biology*, **42**: 5-7.
- Com. 7.** A.S. Holehouse, R.V. Pappu. Encoding phase transitions. (2015). *Nature Materials*. **14**: 1083-1084. Invited News & Views piece.
- Com. 8.** R.V. Pappu (2015). Cell signaling, division, and organization mediated by intrinsically disordered proteins. *Seminars in Cell and Developmental Biology*. **37**: 1-2.
- Com. 9.** R.V. Pappu. (2014). Frozen in Beta. *Biophysical Journal*. **107**: 795-797. Invited New & Notable Piece.
- Com. 10.** A.K. Dunker et al. (2013). What's in a name? Why these proteins are called intrinsically disordered? *Intrinsically Disordered Proteins*. **1**: e24157.
- Com. 11.** 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.
- Com. 12.** R.V. Pappu, R. Nussinov. (2009). Protein folding: Lessons learned and new frontiers. *Physical Biology* **6**: 010301-1. PMID: 19208944.
- Com. 13.** R.V. Pappu. Review of the Fourth Johns Hopkins Protein Folding Meeting. (1999). *Proteins: Structure Function, and Genetics*, **36**: 263-269.

Submitted Manuscripts / preprints

- Sub.-01.** L-P Bergeron-Sandoval, S. Kumar, H.K. Heris, C.L.A. Chang^c, C.E. Cornell^c, S. L. Keller, P. François^d, A.G. Hendricks, A.J. Ehrlicher, R.V. Pappu[†], S. W. Michnick[†]. Proteins with prion-like domains form condensates that are inferred to be viscoelastic and enable membrane remodeling and endocytosis. ([†]Co-corresponding authors). *Proceedings of the National Academy of Sciences USA*, revised version under review.
- Sub.-02.** M.V. Staller, E. Ramirez, A.S. Holehouse, R.V. Pappu, B.A. Cohen. Design principles of acidic activation domains. *Cell Systems*, revisions being prepared following the first round of reviews.
- Sub.-03.** I. Seim, A.E. Posey, W.T. Snead, B.M. Stormo, D. Klotsa, R.V. Pappu[†], A.S.

Gladfelter[†]. ([†]Co-corresponding authors). Negative regulation of a ribonucleoprotein condensate driven by dilute phase oligomerization. *Proceedings of the National Academy of Sciences USA*, revisions being prepared following the first round of reviews.

Sub.-04. S. Jelenic, J. Bindics, P. Czermak, M. Ruer, A.S. Holehouse, **R.V. Pappu**, S. Saha. Complex composition can buffer protein dynamics within liquid-like condensates. *EMBO Journal*, revisions being prepared following the first round of reviews.

Sub.-05. N.S. Gonzalez-Foutel, W.M. Borchers, J. Glavina¹, S. Barrera-Vilarmau, A. Sagar, A. Estaña, A. Barozet, G. Fernandez-Ballester, C. Blanes-Mira, I.E. Sánchez, G. de Prat-Gay, J. Cortés, P. Bernadó, **R.V. Pappu**^{*}, A.S. Holehouse^{*}, G.W. Daughdrill^{*} L.B. Chemes^{*}. (^{*}Co-corresponding authors). Conformational buffering underlies functional selection in intrinsically disordered protein regions. *Nature Structural and Molecular Biology*, revisions being prepared following the first round of reviews.

Sub.-06. M. Kar, A.E. Posey, F. Dar, A.A. Hyman^{*}, **R.V. Pappu**^{*}. (^{*}Co-corresponding authors) Glycine-rich peptides from FUS have an intrinsic ability to self-assemble into fibers and self-supporting hydrogels. *Biochemistry*, revisions being prepared following the first round of reviews.

Sub.-07. M.C. Cohan, M-K. Shinn, J.M. Lalmansingh, **R.V. Pappu**. Uncovering non-random sequence patterns within intrinsically disordered proteins. *Journal of Molecular Biology*, under review.

Sub.-08. K.M. Ruff[§], Y-H. Choi[§], D. Cox, A. Ormsby, Y. Myung, D. B. Ascher, S.E. Radford, **R.V. Pappu**[†], D.M. Hatters[†]. Sequence grammar for phase separation of unfolded states of globular proteins. ([§]Co-first authors; [†]Co-corresponding authors). *Submitted to Molecular Cell*.

Manuscripts in preparation

Prep.01. M.J. Fossat, A.E. Posey, **R.V. Pappu**. Quantifying charge state heterogeneity for proteins with multiple ionizable residues.

Prep.02. M. Kar, F. Dar, T.J. Welsh, A. Pozniakovsky, R. Lemaitre, J. Wang, G. Meisl, S. Alberti, T.P.J. Knowles, A. A. Hyman[†], **R. V. Pappu**[†]. Phase transitions of RNA binding proteins are distinct from conventional liquid-liquid phase separation. ([†]Co-corresponding authors).

Prep.03. X. Zeng, **R.V. Pappu**. Competing interactions give rise to sequence-specific bistable conformational ensembles for intrinsically disordered proteins.

Prep.04. M-K. Shinn[†], M.C. Cohan[†], K.M. Ruff, J.L. Bullock, P. A. Levin, **R.V. Pappu**. Impacts of sequence patterns within the disordered tail of *B. subtilis* FtsZ on assembly and functions. ([†]Co-first authors).

Prep.05. M. Farag, A. Bremer, W.M. Borchers, T. Mittag, **R.V. Pappu**. Experimentally derived stickers-and-spacers model predicts sequence-specific and collective phase behaviors of prion-like low complexity domains.

Prep.06. M.R. King, K.M. Ruff, X. Zeng, A.E. Posey, W. Ouyang, E. Lundberg, **R.V. Pappu**. Nucleolar cores are scaffolded by proteins with lysine and acid-rich disordered regions that drive phase separation.

Prep.07. M. Farag, **R.V. Pappu**. Distinct conformational characteristics underlie the inhomogeneous network structure within and interfacial properties of biomolecular condensates.

- Prep.08.** T. Wu, M.R. King, **R.V. Pappu**, M.D. Lew. Single molecule localization microscopy reveals inhomogeneous network structures of archetypal biomolecular condensates.
- Prep.09.** F. Dar, M. Farag, **R.V. Pappu**. Physics of phase transitions and biomolecular condensates. *For Nature Reviews Physics*.
- Prep.10.** F. Dar, **R.V. Pappu**. Complex phase behaviors of multicomponent systems of macromolecules with sticker-and-spacer architectures.
- Prep.11.** M.J. Fossat, **R.V. Pappu**. Efficient q -canonical Monte Carlo simulations of charge regulation.
- Prep.12.** A.E. Posey[§], M. J. Fossat[§], **R.V. Pappu**. Stabilization of single alpha helices by preferential neutralization of ionizable residues. ([§]Co-first authors).
- Prep.13.** J.M. Lalmansingh, K.M. Ruff, A.T. Keeley, **R.V. Pappu**, A.S. Holehouse[†]. A general-purpose analysis library for analyzing simulations of intrinsically disordered proteins. ([†]Corresponding author).
- Prep.14.** A.Z. Lin, A. E. Posey, M.R. King, F. Dar, A. S. Gladfelter, **R. V. Pappu**. Driving forces for unmixed condensates formed by the multivalent Whi3 protein and distinct RNA molecules.
- Prep.15.** F. Dar[§], J-M. Choi[§] A. Phillips, D. Mitrea, C.B. Stanley, R.W. Kriwacki[†], **R.V. Pappu**[†]. Network-fluid structure and dynamics of biomolecular condensates formed by phase separation of multivalent proteins. ([§]Co-first authors; [†]co-corresponding authors).
- Prep.16.** M.J. Fossat, **R.V. Pappu**. Impact of charge regulation on conformational and phase equilibria of intrinsically disordered proteins. *To be submitted as a feature article to J. Phys. Chem. B*.
- Prep.17.** M. Farag, F. Dar, J.P. Taylor, **R.V. Pappu**. How do topologies of protein-protein interaction networks impact the driving forces for phase separation in multicomponent systems?
- Prep.18.** M. Farag[§], X. Zeng[§], A. Chilkoti, **R.V. Pappu**. Impact of sequence-encoded energetic frustration on the phase behavior of intrinsically disordered proteins. ([§]Co-first authors).
- Prep.19.** X. Zeng, M.J. Fossat, K.M. Ruff, **R.V. Pappu**. Physics of intrinsically disordered proteins. *For Reports on Progress in Physics*.
- Prep.20.** X. Zeng, K.M. Ruff, **R.V. Pappu**. Improving the efficiency and robustness of CAMELOT – a machine-learning methodology for systematic coarse-graining.
- Prep.21.** A.E. Posey[†], M. R. King, **R.V. Pappu**[†]. Experimental methods for mapping coexistence curves of biological macromolecules. ([†]Co-corresponding authors).
- Prep.22.** 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 Institutes of Health, R01NS121114

Title: *Understanding the sequence and structural determinants of phase behavior of ALS causing proteins*

Principal Investigators: Tanja Mittag (St. Jude Children's Research Hospital), Rohit Pappu

Funding period: February 01, 2021 – January 31, 2026

Principal Role in the project: Co-PI in multi-PI grant

Air Force Office of Scientific Research, Multidisciplinary University Research Initiative (MURI), FA9550-20-1-0241 Topic 20: Fundamental Design Principles for Engineering Orthogonal Liquid-Liquid Phase Separations in Living Cells

Title: *Uncovering and applying the interfacial design principles of multiphasic natural and synthetic organelles*

Funding Period: October 01, 2020 – September 30, 2025

Principal Investigators: Clifford P. Brangwynne (contact PI, Princeton University), Jose Avalos (co-PI, Princeton University), Ashutosh Chilkoti (co-PI, Duke University), Amy Gladfelter (co-PI, University of North Carolina), **Rohit Pappu (co-PI, Washington University in St. Louis)**, Lingchong You (co-PI, Duke University)

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, 2021

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 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, 2022

Role in the project: *Principal Investigator*

National Institutes of Health, 1R01NS089932

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

Funding period: April 01, 2016 – December 31, 2021

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

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

PENDING

National Science Foundation, DMR 1729783 – DMREF Collaborative Research

Title: *Expanding the Universe of Materials Based on Intrinsically Disordered Proteins Using High Throughput Experiments and Multiscale Computations*

Principal Investigators: Rohit Pappu (contact PI), Ashutosh Chilkoti Mittag (co-PI), Stefan Zauscher (co-I);

Requested Funding period: October 01, 2021 – September 30, 2025

Role in the project: *Contact Principal Investigator* in collaborative grant

National Institutes of Health (NINDS), 2R01NS056114

Title: *Uncovering the interplay between homotypic and heterotypic interactions on the phase behavior of huntingtin*

Funding period: April 01, 2022 – March 21, 2027

Role in the project: *Principal Investigator*

St. Jude Research Collaborative 2.0, Sponsored by St. Jude Children's Research Hospital,

Title: *Physical underpinnings of the complex biology of RNP granules*

Funding period: February 01, 2022 – January 31, 2027

Role in the project: *Project Principal Investigator*, Material properties of RNP granules, crosstalk among RNP granules, and molecular grammars underlying nucleolar and nuclear speckle organization

COMPLETED

National Science Foundation, MCB-1614766

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

Funding period: July 15, 2016 – July 14, 2021

Role in the project: *Principal Investigator*

Dewpoint Therapeutics, Sponsored Research Agreement

Title: *Cataloging and characterizing biomolecular condensates*

Funding Period: November 01, 2019 – October 31, 2020

Role in the project: *Principal Investigator*

National Institutes of Health, 1R01GM108785

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

Title: *Role of chain length and sequence contexts on polyglutamine oligomerization*

Funding period: July 01, 2011 – June 30, 2016

Role in the project: PI

National Science Foundation, MCB-0718924

Title: *Phase behavior of intrinsically disordered proteins*

Funding period: September 01, 2011 – August 31, 2015

Role in the project: Principal Investigator

National Institutes of Health, 1S10OD018091 Shared Instrumentation Grant

Title: *GPU computing resource to enable innovation in imaging and network biology*

Funding period: April 01, 2014 – March 31, 2015

Role in the project: Co-PI with Fred Prior

National Institutes of Health (NINDS), 5R01NS056114

Title: *Atomistic studies of nucleation and oligomerization in polyglutamine aggregation*

Funding period: April 15, 2007 – June 30, 2012

Role in the project: PI

National Science Foundation, MCB-0718924

Title: *Conformational equilibria of intrinsically disordered proteins*

Funding period: September 01, 2007 – August 31, 2011

Role in the project: PI

Hope Center for Neurological Disorders, Washington University School of Medicine

Translational Neuroscience Pilot Project

Title: *Mechanism of Huntingtin Aggregation Regulated by Profilin*

Funding period: June 01, 2011 – May 31, 2013

Role in the project: Principal Investigator

Co-Investigator: Marc Diamond

National Institutes of Health (NCI) U54 CA-119342

Title: *An informatics resource for targeted nanoparticle therapeutics*

NCI Center grant to the Siteman Center for Cancer Nanotechnology Excellence (Center grant

PI: Samuel Wickline)

Funding period: February 01, 2006 – January 31, 2011

Role in the project: Project Principal Investigator

Project Co-Investigators: David Sept, Nathan Baker

Pfizer Inc., St. Louis, MO

Title: *Modeling the aggregation of therapeutic monoclonal antibodies*

Funding period: October 31, 2009 – September 30, 2010

Role in the project: Project Principal Investigator

National Institutes of Health (NCI) Integrated Cancer Research Workspace 94358NBS23

Subcontract for with Booz Allen Hamilton for Nanotechnology working group

Funding period: April 01, 2008 – February 14, 2009

Role in the project: Principal Investigator

National Science Foundation, MCB-0416766

Title: *Studying the origin of conformational preferences in unfolded proteins*

Funding period: September 01, 2004 – August 31, 2007

Role in the project: Principal Investigator

Hope Center for Neurological Disorders, Washington University School of Medicine

Translational Neuroscience Pilot Project

Title: *Investigation of structural changes induced in amyloid A β 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

RESEARCH MENTORING

Current Postdoctoral and Research Scientists

1. **Martin J. Fossat**, Postdoctoral Scientist
2. **Matthew R. King**, Postdoctoral Scientist
3. **Ammon E. Posey**, Research Scientist
4. **Kiersten M. Ruff**, Research Scientist
5. **Xiangze Zeng**, Postdoctoral Scientist

Current Doctoral Students (alphabetical order)

1. **Furqan Dar**, Doctoral Student, Department of Physics, Projected graduation date, December 2021.
2. **Mina Farag**, MD / PhD Student, Department of Biomedical Engineering, Projected graduation date, Spring 2023.
3. **Jared M. Lalmansingh**, Doctoral Student, Department of Physics. Projected graduation date, May 2021.
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. **Kaitlyn Hardesty**, Undergraduate student in the Department of Biomedical Engineering. Scheduled to graduate, May 2022.

Current Research Staff (alphabetical order)

1. **Catherine Kornacki**, Laboratory Research Technician, August 2019 onward.

Lab alumni – reverse chronological order

1. **Megan C. Cohan**, Doctoral Student, Department of Biomedical Engineering, May 2016 – December 2020.
2. **Max V. Staller**, Co-mentored Postdoctoral Scientist (primary mentor: Barak A. Cohen), March 2015 – December 2020.
3. **Anna M.P. Eddelbuettel**, Undergraduate researcher, May 2018 – May 2020.
4. **Alex S. Holehouse**, Doctoral Student, Computational and Molecular Biophysics, May 2013 – May 2017.
5. **Garrett Ginell**, Junior Computational Research Scientist, August 2018 – August 2019

6. **Jeong-Mo Choi**, Postdoctoral Scientist, August 2016 – April 2019.
7. **Mary O. G. Richardson**, Junior Research Scientist and Scientific Programmer, August 2017 – June 2018.
8. **Sang Eun Jee**, Postdoctoral Scientist, November 2016 – October 2017.
9. **Kourtney L. Kroll**, Undergraduate researcher, Summer 2017.
10. **Divya Natarajan**, MD Student researcher, Washington University School of Medicine, summer 2017.
11. **Tyler S. Harmon**, Doctoral Student, Department of Physics. Received PhD in April 2017. Currently, postdoctoral scientist at the Max Planck Institute in Dresden, Germany.
12. **Rajni Verma**, Postdoctoral Scientist, October 2015 – June 2016.
13. **Rahul K. Das**, Postdoctoral Scientist, September 2009 – August 2015.
14. **Anuradha Mittal**, Postdoctoral Scientist. Currently, a senior Bioinformatics Scientist at Affymetrix, San Francisco, CA.
15. **Laruen M. Bedell**, Undergraduate Student, Department of Biomedical Engineering.
16. **Kanchan Garai**, Research Assistant Professor and Research Scholar, August 2013 – May 2014.
17. **James Ahad**, Undergraduate student, Biomedical Engineering. Currently, an MSTP student at Case Western University School of Medicine.
18. **Scott L. Crick**, Doctoral Student, Biomedical Engineering. Received Ph.D. in August 2011. Completed a two-year Postdoc in the lab in July 2013.
19. **Siddique J. Khan**, Postdoc, April 2012 – May 2013.
20. **Nicholas Lyle**, Doctoral Student, Computational & Systems Biology Program, Division of Biology & Biomedical Sciences. Received Ph.D. in May 2013.
21. **Tony Wang**, Summer undergraduate researcher, Summer 2012.
22. **Marta Wells**, Summer undergraduate research, Summer 2011 and 2012.
23. **Albert H. Mao**, M.D.-Ph.D. student, Computational & Molecular Biophysics Program. Received Ph.D. in August 2012.
24. **Jordan Nick**, Summer HHMI undergraduate fellow, Summer 2011.
25. **Kelly Culhane**, SURF student, Summer 2011. Currently, a Ph.D. student in Biochemistry & Biophysics at Yale University.
26. **Aditya Radhakrishnan**, Master's student (BS/MS), Summer 2010 – Summer 2011.
27. **Nil Gural**, Undergraduate researcher, Spring 2011. Currently Ph.D. student in the Harvard-MIT Health Sciences Program.
28. **Adam T. Steffen**, Scientific programmer, Summer 2007 – December 2010.
29. **Alexander French**, Undergraduate researcher, Summer 2010.
30. **Anil Kumar**, Postdoctoral scientist, December 2009 – August 2010.

31. **Caitlin L. Chicoine**, Undergraduate researcher, Summer of 2009,
32. **Matthew A. Wyczalkowski**, Biomedical Engineering. Received his Ph.D. in December 2009.
33. **Tim E. Williamson**, Molecular Biophysics Program, Division of Biology & Biomedical Sciences and Staff Scientist. Received MS in May 2009.
34. **Andreas Vitalis**, Doctoral Student, Molecular Biophysics Program, Division of Biology & Biomedical Sciences. Received his Ph.D. in June 2009.
35. **Alan A. Chen**, Doctoral Student, Molecular Biophysics Program, Division of Biology & Biomedical Sciences. Received his Ph.D. in May 2009.
36. **Jose Pulido**, Undergraduate Trainee, May 2008 – October 2008.
37. **Xiaoling Wang**, Postdoctoral scientist, September 2004 – February 2008.
38. **Hoang T. Tran**, Doctoral student, Biomedical Engineering. Received Ph.D. in December 2007.
39. **Alexander N. Drozdov**, Postdoctoral Scientist, September 2002 – April 2004.
40. **Magdalena Fus**, Undergraduate Trainee, September 2004 – May 2005.
41. **Tirath Patel**, Undergraduate Trainee, September 2004 – May 2005.

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

- Dr. Matthew R. King, postdoc in the Pappu lab, received the postdoctoral award from the Intrinsically Disordered Proteins subgroup of the US Biophysical society. The award, sponsored by Molecular Kinetics, comes with a cash prize and a speaking engagement at the 2021 Subgroup Symposium as part of the annual meeting of the Biophysical Society.
- Ms. Megan C. Cohan, graduate student in the Pappu lab, received the Ceil M. DeGutis prize in Chemical Biology and Medicinal Chemistry for 2020. This award is given by Washington University in St. Louis in recognition of a graduate student's outstanding contributions to Chemical Biology and Medicinal Chemistry, broadly defined. Ms. Cohan was recognized for her research dedicated to understanding how intrinsically disordered regions (IDRs) might contribute to the molecular functions of bacterial proteins.
- Ms. Anna M.P. Edelbuettel, undergraduate student researcher in the Pappu lab, received the Outstanding Senior Award for Academic Excellence, and the Outstanding Senior Achievement Award from the Department of Biomedical Engineering and Washington University in St. Louis.
- Ms. Anna M.P. Edelbuettel, undergraduate student researcher in the Pappu lab, was awarded a three-year graduate research fellowship from the US National Science Foundation.
- Mr. Furqan Dar, graduate student in the Pappu lab, received a Student Research Achievement Award (SRAA) from the Biopolymers In vivo subgroup for his poster presented at the 2020 Annual Meeting of the Biophysical Society in San Diego, CA.
- Dr. Martin J. Fossat, postdoctoral fellow in the Pappu lab, received an award for best postdoctoral poster at the EMBO Workshop on Intrinsically Disordered Proteins held in Bengaluru, India, December 2019.
- Ms. Megan C. Cohan, graduate student in the Pappu lab, received a \$500 travel award to attend the 3rd Fusion Bacterial Cell Biology Conference in the Bahamas, for February 2020.

- Ms. Megan C. Cohan, graduate student in the Pappu lab, was elected to be the graduate student representative to the council of the Intrinsically Disordered Proteins subgroup of the Biophysical Society for the period between April 01, 2019 and March 31, 2020.
- Dr. Jeong-Mo Choi, postdoctoral fellow in the Pappu lab, received a travel award to attend and present his work at the 63rd Annual Meeting of the Biophysical Society, Baltimore, March 2019.
- Ms. Megan C. Cohan, graduate student in the Pappu lab, was elected to the board of BALSAs for the 2019-2020 period. This is the Biotechnology and Life Sciences Advising Group, which is a non-profit organization “that provides consulting services for a variety of clients, ranging from individual faculty members up through multinational corporations”.
- Mr. Jared Lalmansingh, physics PhD student in the Pappu lab, received Washington University’s 2019 Gerry and Bob Virgil Ethic of Service Award for his contributions to the Young Scientist’s Program, an outreach effort to draw students from the inner cities into science.
- 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.

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, Pls 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. *Physics of Biopolymers*, BME 432 / 532, Fall 2019 onward. Audience: Seniors majoring in Biomedical Engineering, Chemical Engineering, and Mechanical Engineering and PhD students from different disciplines including BME, Biophysics, and Materials Science.
2. *Bioengineering Thermodynamics in Practice*, Laboratory Course, BME 329, Fall 2014 & 2015. Audience: Biomedical Engineering juniors.

3. *Bioengineering Thermodynamics*, BME 320B, Fall 2010 onward. Audience: Biomedical Engineering juniors.
4. *Bioengineering Thermodynamics Recitation*, BME 320A, Fall 2015 onward. Problem solving session. Audience: Biomedical Engineering juniors.
5. *Applied Mathematics for Biomedical Sciences*, Fall 2013. Audience: Graduate students in Biomedical Engineering & quantitative programs in the Division of Biology & Biomedical Sciences.
6. *Chemical Thermodynamics*, ChemE 320 / BME 320, Fall 2008 and 2009. Audience: Chemical Engineering sophomores and Biomedical Engineering juniors.
7. *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.
8. *Principles of Protein Structure*, BME 461, Every Fall starting Fall 2003. Audience: Seniors and graduate students in Biomedical Engineering.
9. *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.
10. *Modeling Biomolecular Systems, Part II*, BME 540, Fall 2004. Audience: Graduate students in Biomedical Engineering, Chemical Engineering, Molecular Biophysics, and Computational Biology.
11. *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.
12. *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 my BME colleagues, thus showcasing my ability to be both visionary and collaborative.

SERVICE

SERVICE

Co-organizer, Condensate Colloquium Series, bi-weekly, virtual series focused on biomolecular condensates, July 2021 – present.

Member, Scientific Advisory Board, UK Biomolecular Condensates: Collaboration for Education, Research and Translation (BioConCERT)

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

Reviewer of grants for Swiss National Science Foundation, ERC grants, BBSRC, and Dutch Science Foundation, and Polish Science Foundation

Regular 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*, *Journal of the American Chemical Society*, *Journal of Chemical Theory and Computation*, *Macromolecules*, *Nature*, *Nature Chemistry*, *Nature Communications*, *Proceedings of the National Academy of Sciences USA*, *PLoS: Computational Biology*, *Science*.

Panelist for review of National Science Foundation SBIR grants, Bioinformatics.

Co-author and contributor to Statement of Significance Petition to form a new Intrinsically Disordered Protein subgroup within the Biophysical Society.

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.