

ROHIT V. PAPPU

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PERSONAL BACKGROUND

Education and training

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

Postdoctoral Scientist, Computational Chemistry and Chemical Physics, 1996-1998
Department of Biochemistry and Molecular Biophysics, Washington University Medical School, St.Louis, MO
Mentor: Professor Jay W. Ponder
Co-Mentor: Garland R. Marshall

Ph.D., Theoretical and 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

Positions

May 2007 onwards: Associate Professor, Department of Biomedical Engineering, Washington University in St.Louis; Adjunct Associate Professor, Department of Biochemistry & Molecular Biophysics, Washington University Medical School; Member & Associate Professor, Center for Computational Biology, Washington University Medical School

June 2002 – May 2007: Assistant Professor, Department of Biochemistry and Molecular Biophysics, Washington University Medical School, *Courtesy Joint Appointment*

May 2002 – June 2007: Member, Center for Computational Biology, Washington University Medical School

September 2001 – May 2007: Assistant Professor, Department of Biomedical Engineering, Washington University in St. Louis

Awards and scholarships

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

Selected to attend NEC Biophysics workshop for physics graduate students, June 1996

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

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

RESEARCH

Publications (reverse chronological order)

1. Wang, X, Vitalis, A, Pappu, RV. Effects of chain length and effective concentration on the spontaneous dimerization of polyglutamine. *In preparation.*
2. Tran, HT, Mao, A, Pappu, RV. On the role of backbone-solvent interactions in determining conformational equilibria of intrinsically disordered polypeptides. *In preparation.*
3. Vitalis, A, Wang, X, Pappu RV. ABSINTH – A novel implicit solvation model for biomolecular simulations. *In preparation.*
4. Wyczalkowski, MA, Vitalis, A, Pappu, RV. How useful is replica exchange for calculating free energies of solvation? *In preparation.*
5. Chen AA, Pappu RV (2007). Parameters of monovalent ions in the AMBER-99 forcefield: Assessment of inaccuracies and proposed improvements. *Journal of Physical Chemistry B*. In press.
6. Pappu RV, Wang X, Vitalis A, Crick SL (2007). A polymer physics perspective on driving forces and mechanisms for protein aggregation. *Archives of Biochemistry and Biophysics*. In press.
7. Vitalis, A, Wang, X, Pappu, RV. (2007). Quantitative characterization of intrinsic disorder in polyglutamine: Insights from analysis based on polymer theories. *Biophysical Journal*, 93: 1923-1937.
8. Chen A, Pappu RV. (2007) Quantitative characterization of ion pairing and cluster formation in strong 1:1 electrolytes. *Journal of Physical Chemistry B*, 111: 6469-6478.
9. Crick, SL, Jayaraman, M, Frieden, C, Wetzel, R, Pappu, RV. (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.
10. Tran, HT, Pappu, RV. (2006). Toward an accurate theoretical framework for describing ensembles for proteins under strongly denaturing conditions. *Biophysical Journal*, 91:1868-1886.

11. Wang, X, Vitalis, A, Wyczalkowski, MA, Pappu, RV. (2006). Characterizing the conformational ensemble of monomeric polyglutamine. *Proteins: Structure, Function, and Bioinformatics*, 63: 297-311.
12. Tran, HT, Wang, X, Pappu, RV. (2005). Reconciling observations of sequence-specific conformational preferences with the generic behavior of denatured proteins. *Biochemistry*, 44: 11369-11380.
13. Patriciu, A, Chirikjian, GS, Pappu, RV. (2004). Analysis of conformational dependence of mass-metric tensor determinants in serial polymers with constraints. *Journal of Chemical Physics*, 121: 12708-12721.
14. Drozdov, AN, Grossfield, A, Pappu, RV. (2004). Role of hydration in determining the conformational preferences of alanine dipeptide. *Journal of the American Chemical Society*, 126: 2574-2581.
15. Pappu RV, Rose GD. (2002). A simple model for poly-proline II structure in unfolded states of alanine-based peptides. *Protein Science*, 11: 2437-2455.
16. Pappu RV, Srinivasan R, Rose GD. (2000). The Flory isolated-pair hypothesis is not valid for polypeptide chains. Implications for polypeptide unfolded states. *Proceedings of the National Academy of Sciences USA*, 97: 12565-12571.
17. Hart RK, Pappu RV, Ponder JW. (2000) Exploring the similarities between potential smoothing and simulated annealing. *Journal of Computational Chemistry*, 21: 531-552.
18. Pappu RV. (1999). Review of the Fourth Johns Hopkins Protein Folding Meeting. *Proteins: Structure, Function, Genetics*. 36: 263-269.
19. Pappu RV, Marshall GR, Ponder JW. (1999). A potential smoothing algorithm accurately predicts transmembrane helix packing. *Nature Structural Biology*, 6:50-55.
20. Pappu RV, Hart RK, Ponder JW. (1998). Analysis and application of potential energy smoothing for global optimization. *Journal of Physical Chemistry B.*, 102: 9725-9742.
21. Huang ES, Koehl P, Levitt M, Pappu RV and Ponder, JW. (1998) Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods. *Proteins: Structure, Function, Genetics*, 33: 204-217.
22. Pappu, RV and Weaver, DL. (1998). The early folding kinetics of apomyoglobin. *Protein Science*, 7: 480-490.
23. Pappu RV, Schneller WJ, Weaver DL (1996). Electrostatic Multipole Representation of a Polypeptide Chain: An algorithm for efficient simulation of polypeptide properties. *Journal of Computational Chemistry*, 17: 1033-1055.

Invited talks: Fall 2001 – present (reverse chronological order, includes talks currently scheduled)

1. International Conference on Protein Assembly in Materials, Biology, and Medicine, Crete, Greece, July 2007.
2. Gordon Research Conference: Proteins, Scheduled for June 2007, Holderness, New Hampshire.
3. University of Oregon, Department of Chemistry, November 2007.

4. Washington University in St.Louis, Biophysical Evening Series, December 2007.
5. University of California in Santa Barbara, Department of Chemistry, April 2007.
6. Rice University, Department of Chemistry, March 2007.
7. University of Delaware, Department of Chemistry and Biochemistry, April 2007.
8. Indiana University, Computational Biology and Bioinformatics, September 2006.
9. National Cancer Institute, Frederick, August 2006.
10. FASEB Amyloid Meeting, Snowmass, Colorado, June 2006.
11. DIMACS Workshop on Computational / Experimental Approaches to Protein Defects in Human Disease, Rutgers University, April 2006.
12. University of North Carolina, Chapel Hill, Department of Chemistry, April 2006.
13. Duke University, Department of Biochemistry, April 2006.
14. UTMB, Galveston, TX, Sealy Center for Structural Biology, April 2006.
15. Johns Hopkins University, Department of Chemistry, March 2006.
16. Stanford University, Department of Chemistry, March 2006.
17. I2CAM Exploratory Workshop on Protein Aggregation and Amyloid Formation in Systemic and Neurodegenerative Diseases: Physical, Molecular, and Biological Approaches, EPFL, Lausanne, Switzerland, July 2005.
18. 18th Annual Gibbs Conference on Biothermodynamics, Carbondale IL, October 2004.
19. University of Iowa, Department of Chemistry, Iowa City, May 2004.
20. Washington University, Alzheimer's disease Research Center, April 2004.
21. Washington University, Department of Genetics, October 2002.
22. Washington University, Alzheimer's disease Research Center, December 2002.
23. Washington University, Biophysical Evening Seminar Series, December 2001.
24. University of North Carolina, Biochemistry & Biophysics, January 2001.
25. University of California in Santa Barbara, January 2001.
26. Johns Hopkins University, Biophysical Evening Series, December 2000.
27. Johns Hopkins University, Biophysics & Biophysical Chemistry, November 1998.
28. The Scripps Research Institute, Molecular Biology, March 1996.

SERVICE

Professional activities

1. Reviewer of manuscripts for the *Journal of the American Chemical Society*, *Proteins:Structure, Function, and Genetics*, *Protein Science*, *Biophysical Journal*, *Biophysical Chemistry*, *Journal of*

Chemical Physics, Biomacromolecules, Journal of Molecular Biology, Journal of Physical Chemistry B, and Journal of Computational Chemistry

2. Panelist for review of National Science Foundation SBIR grants, Bioinformatics
3. Ad hoc 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. Member, NIH study section, Biophysics of Neuronal Systems, BPNS, June 2006 – present
9. Primary organizer of 1st International ICAM workshop on Multiscale Interactions and Dynamics in Complex Biological Systems, Washington University in St.Louis, May 27-29, 2006.
10. Co-organizer for 20th Annual Gibbs Meeting on Biothermodynamics, October 7-10, 2006, Carbondale, IL.

Professional society memberships

American Association for Advancement of Science

American Chemical Society

American Physical Society

Biomedical Engineering Society

Biophysical Society

Protein Society