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Education

Ph.D. in Physics & Biochemistry, 2002. Michigan State University, East Lansing, MI
Thesis: "Protein Rigidity and Flexibility: Applications to Folding and Thermostability."

M.S. in Physics, 1998. Michigan State University, East Lansing, MI

B.S. Honors in Physics & Mathematics, 1996. University of Houston, Houston, TX
Graduated *Summa Cum Laude* with Honors in Major and University Honors
Thesis: "Improved Efficiencies in InP/InGaAs Solar Cells by an Anti-reflection Coating Process."

Publications

1. A.J. Rader, Chakra Chennubhotla, Lee Wei Yang, and Ivet Bahar. The Gaussian Network Model: Theory and Applications *to be published* in Normal Mode Analysis: Theory and Applications to Biological and Chemical Systems. CRC Press.
2. A.J. Rader, Daniel H. Vlad, and Ivet Bahar, Maturation Dynamics of Bacteriophage HK97 Capsid, *Structure*, (*in press*).
3. M.F. Thorpe, Mykyta Chubynsky, Brandon Hespenheide, Scott Menor, Donald J. Jacobs, Leslie A. Kuhn, Maria I. Zavodszky, Ming Lei, A.J. Rader, and Walter Whiteley, Flexibility in Biomolecules in the Sir Roger Elliott Festschrift *to be published* by Imperial College Press, London.
4. Mykyta Chubynsky, Brandon Hespenheide, Donald J. Jacobs, Leslie A. Kuhn, Ming Lei, Scott Menor, A.J. Rader, M.F. Thorpe, Walter Whiteley, and Maria I. Zavodszky, Constraint Theory applied to Proteins *to be published* in the Proceedings of the Indo-US workshop, 2004 by Nova Publishers.
5. Yongmei Wang, A.J. Rader, Ivet Bahar, and Robert L. Jernigan, Global Ribosome Motions Revealed with Elastic Network Model, *Journal of Structural Biology* **147**(3), (2004), 302-314.
6. A.J. Rader, Gülsüm Anderson, Basak Isin, H. Gobind Khorana, Ivet Bahar and Judith Klein-Seetharaman, Identification of Core Amino Acids Stabilizing Rhodopsin, *Proceedings of the National Academy of Sciences (USA)* **101**(19), (2004), 7246-7251.
7. A.J. Rader and Ivet Bahar, Folding Core Predictions from Network Models of Proteins, *Polymer* **45**(2), (2004), 659-668.

8. Brandon M. Hesperheide, [A.J. Rader](#), M.F. Thorpe, and Leslie A. Kuhn, Identifying Protein Folding Cores from the Evolution of Flexible Regions during Unfolding, *Journal of Molecular Graphics & Modelling* **21**, (2002), 195-207.
9. [A.J. Rader](#), Brandon M. Hesperheide, L.A. Kuhn, and M.F. Thorpe, Protein Unfolding: Rigidity Lost, *Proceedings of the National Academy of Sciences (USA)* **99**, (2002), 3540-3545.
10. D.J. Jacobs, [A.J. Rader](#), Leslie A. Kuhn, and M.F. Thorpe, Protein Flexibility Predictions Using Graph Theory, *PROTEINS: Structure, Function and Genetics* **44**, (2001), 150-165 (***cover figure**).
11. M.F. Thorpe, Ming Lei, [A.J. Rader](#), Donald J. Jacobs and Leslie A. Kuhn, Protein Flexibility and Dynamics using Constraint Theory, *Journal of Molecular Graphics & Modelling* **19**, (2001), 60-69.
12. M.F. Thorpe, D.J. Jacobs, N.V. Chubynsky & [A.J. Rader](#), Generic Rigidity of Network Glasses in *Rigidity Theory and Applications*, Edited by M.F. Thorpe and P.M. Duxbury. Kluwer Academic/Plenum Publishing, New York (1999) 239-277.
13. D.S. Bracken, K. Kwiatkowski, K.B. Morley, E. Renshaw Foxford, K. Komisarck, [A.J. Rader](#), & V.E. Viola, Charging Effects in Passivated Silicon Detectors, *Nuclear Instruments and Methods in Physics Research A* **365**, (1995) 424-426.

Talks

1. [A.J. Rader](#), "Protein Flexibility, Dynamics, and Folding: Insights from Network Models" University at Buffalo, SUNY, Department of Physics, Buffalo, NY, March 3, 2005.
2. [A.J. Rader](#), "Protein Flexibility, Dynamics, and Folding: Insights from Network Models" University of Pittsburgh, Department of Computational Biology, Pittsburgh, PA, January 24, 2005.
3. [A.J. Rader](#), "Protein Conformation Pathway Generation Using Iterative Elastic Network Models" 2nd Biological Language Conference, Carnegie Mellon University and University of Pittsburgh, Pittsburgh, PA, November 18-19, 2004.
4. [A.J. Rader](#), "Simulating Viral Capsid Maturation Using Elastic Network Models" Computational Methodology in Modeling Complex Biological Systems Workshop, Pittsburgh Center for Biomedical Computation, Pittsburgh, PA, October 13, 2004.
5. [A.J. Rader](#), "Protein Folding Predictions from Network Models" Condensed Matter & Biological Physics Seminar, Department of Physics, Syracuse University, Syracuse, NY, September 24, 2004.
6. [A.J. Rader](#), "Modeling of Bigger Biomolecules & Assemblies" Workshop on Modeling Protein Stability, Flexibility and Motions, Banff, Alberta, Canada, July 17-22, 2004.
7. [A.J. Rader](#), "FIRST and Protein Unfolding" Workshop on Modeling Protein Stability Flexibility and Motions, Banff, Alberta, Canada, July 17-22, 2004.
8. [A.J. Rader](#), "Perspectives on Protein (un)Folding from Rigidity" American Mathematical Society 2004 Spring Eastern Section Meeting, Rider University, Lawrenceville, NJ, April 17, 2004.

9. A.J. Rader, Yongmei Wang, Ivet Bahar, and Robert L. Jernigan, "Motions and Deformations in Ribosome" Biophysical Society 48th Annual Meeting, Baltimore, MD, February 16, 2004.
10. A.J. Rader, "Extensions of FIRST to Nucleotides" Arizona State University, Tempe, AZ, January 30, 2004.
11. A.J. Rader, Gülsüm Anderson, Basak Isin, Judith Klein-Seetharaman, and Ivet Bahar, "The Folding Core in Rhodopsin" Biological Language Conference, Carnegie Mellon University and University of Pittsburgh, Pittsburgh, PA, November 20-21, 2003.
12. A.J. Rader, "Protein Rigidity and Flexibility: Applications to Folding" 2nd Biological Language Modeling Workshop, Carnegie Mellon University, Pittsburgh, PA, May 14, 2003.
13. A.J. Rader, Brandon M. Hespeneide, Leslie A. Kuhn, M.F. Thorpe, "Protein Unfolding: Rigidity Lost" American Physical Society March Meeting, Austin, TX, March 4, 2003.
14. A.J. Rader, "Protein Rigidity and Flexibility: Applications to Folding and Thermostability" T-10 Theoretical Biology & Biophysics Division, Los Alamos National Laboratory, Los Alamos, NM, October 15, 2002.
15. A.J. Rader, "Protein Rigidity and Flexibility: Applications to Folding and Thermostability" Center for Computational Biology & Bioinformatics, University of Pittsburgh, Pittsburgh, PA, October 4, 2002.
16. A.J. Rader, "Protein Unfolding: Rigidity Lost" Condensed Matter Physics Brown Bag Seminar, Department of Physics & Astronomy, Michigan State University, East Lansing, MI, September 27, 2001.
17. A.J. Rader, "The Protein Folding Problem" Condensed Matter Physics Brown Bag Seminar, Department of Physics & Astronomy, Michigan State University, East Lansing, MI, October 12, 2000.
18. A.J. Rader, D.J. Jacobs, and M.F. Thorpe, "Computational Analysis for Random Bond Model Rigidity Percolation" American Physical Society Centennial Meeting, Atlanta, GA, March 26, 1999.
19. A.J. Rader, K. Kwiatkowski, and V.E. Viola, "Leakage Current Effects in Passivated Silicon Detectors" 5th Annual Argonne Symposium for Undergraduates in Science, Engineering, and Mathematics. Argonne National Laboratory, Argonne, IL, November 4-5, 1994.

Posters

- A.J. Rader, Daniel H. Vlad, Yongmei Wang and Ivet Bahar, *Elastic Network Models Reveal Maturation Dynamics of Bacteriophage HK97* Poster at Biophysical Society 49th Annual Meeting, Long Beach, CA, February 2005.
- A.J. Rader, Gülsüm Anderson, Basak Isin, Judith Klein-Seetharaman, and Ivet Bahar *The Folding Core of the G-Protein-Coupled Receptor Rhodopsin* Poster at Biophysical Society 48th Annual Meeting, Baltimore, MD, February 2004.
- A.J. Rader and Ivet Bahar *Folding Core Predictions from Network Models of Proteins* Poster at 35th Central Regional Meeting of the American Chemical Society, Pittsburgh, PA, October 2003.

- A.J. Rader, Basak Isin, Gülsüm Anderson, Judith Klein-Seetharaman, and Ivet Bahar *The Folding Core of the G-Protein-Coupled Receptor Rhodopsin* Poster at Science 2003, University of Pittsburgh, Pittsburgh, PA, September 2003.
- A.J. Rader and Ivet Bahar *Folding Core Predictions from Network Models of Proteins* Poster at UB-SUNY 1st Frontiers in Bioinformatics Symposium, Buffalo, NY, June 2003.
- A.J. Rader, B.M. Hesperheide, L.A. Kuhn, and M.F. Thorpe, *Protein Unfolding Driven by Changing Mean Coordination* Poster at the Protein Society Symposium, San Diego, CA, August 2002.
- A.J. Rader, B.M. Hesperheide, L.A. Kuhn, and M.F. Thorpe, *Protein Unfolding Driven by Changing Mean Coordination* Poster at the MSU Center for Biological Modeling Annual Symposium, East Lansing, MI, June 2002.
- A.J. Rader, B.M. Hesperheide, L.A. Kuhn, and M.F. Thorpe, *The Mean Coordination, $\langle r \rangle$, as a Protein Folding Reaction Coordinate* Poster at the 16th Annual MSU Center for Fundamental Materials Research Symposium, East Lansing, MI, April 2002.
- A.J. Rader, B.M. Hesperheide, L.A. Kuhn, and M.F. Thorpe, *Protein Unfolding: Rigidity Lost?* Poster at the Center for Biological Modeling Annual Retreat, Augusta, MI, May 2001.
- A.J. Rader, L.A. Kuhn, B.M. Hesperheide and M.F. Thorpe; *Protein Unfolding: An Example of a Rigid--Floppy Phase Transition* Poster at the 15th Annual CFMR Symposium, MSU, East Lansing, MI, March 26, 2001.
- A.J. Rader, L.A. Kuhn, B.M. Hesperheide and M.F. Thorpe; *The Transition Between Rigidity and Flexibility in Proteins and Glasses* Poster at the MSU sponsored Protein Flexibility & Folding Workshop, Traverse City, MI, August 13-17, 2000.
- A.J. Rader, L.A. Kuhn, and M.F. Thorpe; *Computational Detection and Analysis of Proteins Flexibility* Poster at the 14th Annual CFMR Symposium, MSU, East Lansing, MI, February 2000.
- A.J. Rader, L.A. Kuhn, and M.F. Thorpe *Prediction of Protein Flexibility* Poster at LJIS Quantitative Challenges in the Post-Genomic Sequence Era: Workshop and Symposium, San Diego, CA, January 2000.
- A.J. Rader and M.F. Thorpe *Ligand Binding Effects on Protein Rigidity and Flexibility* Poster at the 47th Annual Midwest Solid State Conference, Ohio University, Athens, OH, September 1999.
- A.J. Rader, D.J. Jacobs, M.F. Thorpe, & L.A. Kuhn *Rigid and Flexible Regions in Proteins* Poster at the 13th Annual CFMR Symposium, MSU, East Lansing, MI, 1999.
- N.V. Chubynsky, A.J. Rader, D.J. Jacobs and M.F. Thorpe *Bethe Lattice Model of Rigidity Percolation in Glasses* Poster (co-presented with N.V. Chubynsky) at the 46th Annual Midwest Solid State Conference, Iowa State University, Ames, IA, 1998.

Professional Experience

- **2003 – present** **Research Associate with Ivet Bahar**

Department of Computational Biology, University of Pittsburgh School of Medicine (prior to 11/2004 this appointment was through the Center for Computational Biology and Bioinformatics and Department of Molecular Biology and Biochemistry)
 Investigated the dynamics of large structures and assemblies by physically inspired network models. Compared the results from various elastic network models and constraint network models to understand protein folding, structure, dynamics and

function. Identified the folding cores for a series of proteins in agreement with data from hydrogen exchange experiments. Enhanced the FIRST software to model DNA/RNA/protein complexes. Calculated flexibility, rigidity and motions on residue and atomic scales for 70S ribosome. Calculated dynamics contributing to potential maturation pathway for the 110,000 residue HK97 bacteriophage virus capsid. Applied computational techniques to propose a plausible folding pathway for the prototypical G-protein-coupled receptor, rhodopsin. Collaborated with Dr. Judith Klein-Seetharaman's lab to investigate membrane protein folding pathways. Interpreted UV Raman resonance spectroscopy of a small protein, trpcage, in terms of unfolding dynamics observed in MD simulations. In many of these projects, I conducted my own research as well as supervising the work of several graduate students.

- **1998 – 2002 Research Assistant with Michael F. Thorpe and Leslie A. Kuhn**

Department of Physics and Astronomy and Department of Biochemistry and Molecular Biology, Michigan State University

Developed theoretical and computational techniques to model and predict the flexibility of proteins, which resulted in the FIRST software (<http://firstweb.asu.edu>). Studied rigidity percolation in network glasses and proteins. Defined a protein unfolding reaction coordinate and connected protein unfolding to increasing flexibility. Investigated the structural flexibility of numerous proteins. Suggested a relationship between thermostability and rigidity in families of homologous proteins. Acquired a working knowledge of protein-ligand interactions, molecular modeling, and numerical methods within the context of interdisciplinary scientific inquiry by collaborating with researchers from biochemistry, computer science, and mathematics.

- **1996-1997, 2001 Teaching Assistant**

Department of Physics and Astronomy, Michigan State University

Taught undergraduate physics courses and labs covering mechanics, thermodynamics, and optics on introductory and advanced levels. Developed quiz and exam questions, conducted recitation periods, directed laboratory experiments, met with students upon request, and graded written work.

- **1994 – 1996 Research Assistant with Alex Freundlich**

Department of Physics and Space Vacuum Epitaxy Center, University of Houston

Fabricated and tested tunnel junction and photovoltaic devices. Implemented an anti-reflection coating procedure and modeled dependence of efficiency on multi-layer thicknesses.

- **Summer 1994 Research Assistant with Victor Viola and Kris Kwiatkowski**

Indiana University Cyclotron Facility, NSF-REU summer program

Tested and corrected leakage current voltage in ISIS semiconductor detectors.

Awards

- Young Investigator's Scholarship, University of Buffalo-SUNY Frontiers in Bioinformatics Symposium, 2003
- Thomas Kaplan Award for best CMP Graduate Research Presentation, Michigan State University Physics Dept., 2001–2002

- Center for Biological Modeling Graduate Award, Michigan State University, 2000 & 2001
- Herbert T. Graham Scholarship, Michigan State University, 1998
- Arete Award (outstanding senior thesis), University of Houston, 1996
- H. Gordon and Bernice Davis Memorial Scholarship, University of Houston, 1995–1996
- National Merit Scholar, University of Houston, 1992–1996

Computational Skills

- Programming languages: FORTRAN, C/C++, perl, HTML, LaTeX.
- I helped write, maintain and update the source code for the FIRST software (<http://www.bch.msu.edu/labs/kuhn/web/projects/first/home.html>) and its web version: <http://firstweb.asu.edu>.
- Experience with molecular modeling and dynamics software: rasmol, InsightII, VMD, NAMD, and MOIL.

Professional Affiliations

American Physical Society, Biophysical Society & Protein Society