

Robert L. Jernigan

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Education

- 1963* – B.S. in Chemistry, California Institute of Technology
- 1968* – Ph.D. in Chemistry, Stanford University
Thesis on Statistical Mechanics of Polymers.
Advisor: P. J. Flory (Nobel Laureate)
- 1968* – Postdoctoral Fellow, Stanford University, with P. J. Flory
- 1968 – 1970* NIH Postdoctoral Fellow, University of California, San Diego, with B. H. Zimm
- 1970 – 1974* Senior Staff Fellow, Physical Sciences Laboratory, Division of Computer Research and Technology, National Institutes of Health
- 1974 – 1975* Senior Staff Fellow, Laboratory of Theoretical Biology, National Cancer Institute, National Institutes of Health

Professional Positions

- 1975 – 2002* Physical Chemist, Laboratory of Experimental and Computational Biology, National Cancer Institute, National Institutes of Health
- 1989 – 2002* Deputy Chief, Laboratory of Experimental and Computational Biology, NIH
- 1992 – 2002* Chief, Section on Molecular Structure, NIH
- 2002 – 2016* Director, Laurence H. Baker Center for Bioinformatics and Biological Statistics, Iowa State University
- 2002 – Pres.* Charles F. Curtiss Distinguished Professor in Agriculture and Life Sciences, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University
- 2012 – Pres.* Affiliate Professor, Department of Physics, Iowa State University
- 2013 – Pres.* Affiliate Professor, Department of Computer Science, Iowa State University

Committees

- 1984 – 1988* Chairman, NIH Advisory Committee on Computer Usage
- 1989 – 2002* Time Allocation Group for supercomputer time at the Advanced Scientific Computing Laboratory, FCRDC, Frederick

- 1989 – 2002 NCI-Advanced Scientific Computing Laboratory
Coordination Group
- 1993 – 1998, 2000 – 2002 NIH Inter-Institute Structural Biology
Steering Group
- 1993 – 2002 Resource Advisory Committee for Parallel Processing
Resource, Cornell University Theory Center
- 1994 – Award Committee – Biophysical Society
- 1995 – 1997 NIH Telecommunications Committee
- 2001 – 2007 Publications Committee, Biophysical Society overseeing
Biophysical Journal
- 2003 – 2007 Chairman, Publications Committee, Biophysical Society
- 2002 – 2015 Plant Sciences Institute Council, Iowa State University
- 2002 – Pres. Supervisory Committee, Bioinformatics and
Computational Biology Program
- 2003– Pres. Biochemistry, Biophysics and Molecular Biology
Department – Computing Committee
- 2005 – National Advisory Committee, Minnesota Supercomputing
Institute, Univ. Minn.
- 2005 – 2010 External Advisory Committee, Tuskegee University (NSF
HBCU-HP)
- 2004 – Pres. Departmental Promotion and Tenure Committee
- 2007 – 2016. Research Computing Council (ISU)
- 2008 – Program Committee for Intelligent Systems for Molecular
Biology
- 2008- 2011 Program Committee for European Conference on
Computational Biology
- 2009 – 2011 Program Committee International Society for
Computational Biology
- 2010 – 2016 ISU Steering Committee for Interdisciplinary Applied
Scientific Computation
- 2010 – 2016 Member, Advisory Board, New Mexico State University,
CREST Center for Bioinformatics and Computational Biology
- 2010 – 2016 Member, Advisory Committee on Bioinformatics, George
Washington University
- 2010, 2011 – Chair, National Academy, Molecular Dynamics ANTON
Award Committee
- 2011 – ISU Steering Committee on High Performance Computing
- 2014 – Department of Mathematics, Iowa State University, Search
Committee for Mathematical Biology
- 2018-2022 Chair, Admissions Committee, Bioinformatics and
Computational Biology Program, ISU

2019-Pres. Promotion Committee Biochemistry, Biophysics, and
Molecular Biology Departments

2021-Pres. Distinguished Professor Review Committee

Present – Program of Study Committees – 10 graduate students

**Professional
Memberships**

American Association for the Advancement of Science
American Chemical Society
Biophysical Society
Protein Society
American Society for Biochemistry and Molecular Biology
RNA Society
International Society for Computational Biology

**Current editorial
boards**

Bioinformatics and Biological Insights
Journal of Data Mining in Genomics & Proteomics

Awards

NIH Postdoctoral Fellowship
NIH Special Achievement Cash Award, 1982
EEO Officers Recognition Award, 1993
NIH Merit Award *”in recognition of research contributions on protein and nucleic acid structures leading to deeper comprehension of conformations and biological functions,”* 1995
Fellow, The Institute for Advanced Studies, Hebrew University, Jerusalem, 1998-1999
Fellow, AAAS, 1999
Top 5% of NIH intramural supported researchers, 2008
Iowa State University Award for Excellence in Research, 2008
Fellow, Biophysical Society, 2009
Gamma Sigma Delta Faculty Honor Society, Iowa State University, 2011
Outstanding Research Award, College of Agriculture and Life Sciences, Iowa State University, 2016
PROSE Award for best textbook in the biological and life sciences, 2018
Regents Award for Faculty Excellence, Iowa State University, 2019
Charles F. Curtiss Distinguished Professor in Agriculture and Life Sciences and Professor, 2020

Grants

NIH Intramural Targeted Anti-Viral AIDS Program Calculations of Preferred Ligands of the HIV-1 Protease Surface, 1990-2
NIH Intramural Targeted Anti-Viral AIDS Program Enzyme Binding Sites for Peptides, 1992-4
United States-Israel Binational Science Foundation - Structure and Sequence Variability Evaluated with a Computer- Vision Method (#91-00219) 1992-5 (with R. Nussinov)
NIH Intramural Targeted Anti-Viral AIDS Program for Improving Peptide Inhibitors for Receptor Targets, 1994-6
NATO Collaborative Research Grants Programme, 1996-7 (with I. Bahar)

United States-Israel Binational Science Foundation – Probing Immunoglobulin Polyreactivity via Highly Efficient Docking, Fold Recognition and Kinetics 1997-2000 (with R. Nussinov and H. Woolfson)
US Army Breast Cancer – Deriving Structures for Lead Drug Discovery from Cell-Line Screens, 1998-2001
NIH-NSF BBSI: Summer Institute in Bioinformatics and Computational Biology, 2002-6
NIH R21 – Discovering Protein Sequence Structure Function Relationships, 2003-7
Sun Microsystems – Academic Equipment, 2004
NSF – CNS MRI – Acquisition of a 512-node BlueGene/L Supercomputer for Large-Scale Applications in Genomics and Systems Biology, 2005-8
ISU – Center for Integrated Animal Genomics – Comparative Genomics to Improve Livestock Gene Annotations, 2007-9
NIH-NSF Grant – BBSI: Summer Institute in Bioinformatics and Computational Systems Biology, 2006-10
DOE – Nanoimaging to Prevent and Treat Alzheimer’s Disease, 2008-10
NIH R01 – High-Accuracy Protein Models Derived from Lower Resolution Data
NSF-MCB Structural Interpretation of Protein Interactomes, 2010-2016
NIH R01 Coarse Grained Proteins (2009-2014)
NIH R01 Modeling Ribosomal Control, Function and Assembly, 2006-2013
NSF MCB Structural Interpretation of Protein Interactomes
USDA Hatch Act Salary Support – Project – Structural and Functional Genomics, 2006-
NIH-NIAID Structure and Mechanism of the AbgT-family Transporters, 2015-2018
NSF-PHY Mechanical Responses at Intercellular Junctions, 2016-2019
NSF-ABI Innovation: Computational Identification & Screening for Deleterious Mutants 2017-2019
NSF Defining the architecture of the Pyk2 activation complex, 2017-2022
NIH-NIGMS Protein Sequence Matching 2018-2022
NSF-MCB Defining the structural organization of the polysaccharide-synthesizing multiprotein complexes localized in Golgi 2019-2023
NIH-HGRI Novel Use of Genome Information to Understand Mutations 2021-2026
NIH-NIGMS Statistical Methods for Higher Order Dependencies to Understand Protein Functions 2021-2024
DOE Novel Systems Approach for Rational Engineering of Robust Microbial Metabolic Pathways 2021-2024

Research Fields

Bioinformatics
Datamining
Simulation Science
Genomics
Bioengineering
Computational Chemistry
Computational Biology
Structural Biology
Biophysics
Mathematical Biology
Systems Biology
Machine Learning
Phylogenies
Evolution

Precision Medicine

Current Research Topics

Datamining to Understand Biological Complexity

Combining Diverse Data

Bringing basic knowledge of protein mechanisms to enable the identification of aberrant mutants

Improving protein sequence matching by including information about protein structures and mechanisms

Applying simulations to interpret single molecule experiments

Developing mechanisms for molecular machines

Updating gene annotations based on new protein sequence matching

Improving protein/gene annotations by using large protein language model data

Tools to identify deleterious mutants in RNA-Seq, proteomics and genomic data

Annotating human genes and other organism genomes

Identifying compensatory mutations to restore function

Phylogenies for evolution and virus progression

New Molecular-based Therapies

Research Topics

Molecular Computations and Simulations

Molecular Modeling

Drug Selection

Genome Comparisons

Mutation Evaluations

Datamining

Multi-Scale Modeling

Biomolecular Dynamics for Functional Mechanisms

Protein Design to Control Function

Molecular Mechanisms

Cell Imaging

Cell Simulations

Building Molecular Machines

Improved Sequence Matching Using Structural Information

Analyses of Complex Biological Data

Protein Evolution

Protein Annotation

Genome to Phenome Mapping

Precision Medicine

Interests

Elucidation of molecular details of biochemical and biophysical processes through the study of macromolecular conformations

Computer modeling and simulations

Development of coarse-grained approaches to overcome sparse data

Protein and Cell Engineering

Drug design

Developing a combined experimental and theoretical methods to elucidate structures of proteins and nucleic acids

Computer simulations of protein and RNA folding. Conformation enumeration of all chain tracings in restricted space within a given shape

Effects of external conditions, including solvent and temperature, on the relative stabilities of macromolecular conformations
Molecular interactions, recognition and specificity
Nucleic acid conformational properties and their relationship to function, recombination and regulation
Utilizing sequence similarities directly in conformational calculations
Conformational transitions between ordered and disordered states, and between various ordered states
Animating organelle images
Molecular visualization
Dynamics of complex molecular assemblages, with the goal of constructing models of cellular processes such as mitosis
Using protein interaction data to construct molecular machines
Understanding protein sequence through structure
Gene annotation through structural modeling
Genome comparisons
Frameworks for combining diverse types of data

Scientific
Accomplishments

Methods for averaging over conformations of flexible macromolecules
Dynamic programming to choose optimum combination of protein secondary structures
Matrix methods for calculating physical properties
Equilibrium pathway model for protein folding
Coarse-graining of structures
Residue-residue interaction energies for proteins
Demonstration of weaker base pairings within promoter sequences
Sequence-dependent conformational fluctuations for different DNA sequences
Calculation of sequence dependence of DNA double helix preferences
Generating and counting large numbers of diverse chain tracings for proteins and nucleic acids
Demonstration that intra-molecular interactions and solvation effects favor observed sequence dependences of DNA double helix groove variabilities
Derivation of amino acid substitution matrix from crystal structures
Treating RNA folding in three dimensions by generating chain tracings on lattice points
Treating peptide binding to surfaces of other macromolecules by generating peptide conformations on neighboring lattice sites
Modeling the bending of nucleic acid double helices around proteins
Discovery of high regularity of coordination geometry of protein ligands around cations
Established correlations between fluctuations in coarse-grained proteins and X-ray temperature factors and hydrogen exchange protection
Development of lattices from observed packing in protein crystals
Elastic networks and normal mode analyses to identify functional motions of coarse-grained proteins
Development of methods to calculate large scale motions in very large structures
Establishing a mechanistic connection between large scale motions in Reverse Transcriptase and the nucleic acid processing steps
Identifying “wobble” motions in tubulin, related to its behavior
Identifying internal cavity changes in GroEL/GroES that assist protein unfolding
Identifying critical motions of the ribosome and relating them to translocation
Comprehending the highly coordinated motions of the ribosome in its mechanism

Networks as unifying models in biology
Development of methods to extract dynamics from sets of crystal structures
Methods to treat explosive exothermic reactions and their ballistics, e.g., ATP hydrolysis
Interpreting the effects of force on cadherins between interacting cells
Datamining protein structures to obtain protein entropies
Major improvements to protein sequence matching by including structural information
Major gains in annotation specificity from new protein sequence matching and from the use of large protein language models
Annotation of all human proteins previously having unknown functions
Improved phylogenies based on homology scores

Meetings Organized

2003 – Organizing Committee, 13th Conversation in Biomolecular Stereodynamics
2004 – Iowa Bioinformatics Workshop
2005 – Organizing Committee, 14th Conversation in Biomolecular Stereodynamics
2005 – Iowa Bioinformatics Workshop
2005 – Integration of Structural and Functional Genomic, ISU
2006 – Steenbock Symposium on Dynamics of Proteins and Macromolecular Assemblies, Madison, WI
2009 – Systems Biology: Integrative, Comparative and Multi-Scale Modeling at Iowa State University
2009 – Iowa State University Bioinformatics Research Fair
2010 – RNA in Motion, ISU
2010 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
2011 – Zing Conference – Protein and RNA Structure Prediction Conference, Mexico
2012 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
2013 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
2013 – Zing Conference – Protein and RNA Structure Prediction Conference, Mexico
2014 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
2014 – Zing Conference on Protein Folding, Dominican Republic
2016 – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
2016 - First International Conference on Computational Genetics and Proteomics, Guanacaste
2017 – Second International Conference on Computational Genetics and Proteomics, Panama
2017 - 4th International Conference on Protein & RNA Structure Prediction, Montego Bay, Jamaica
2018 - Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
2019 - Biomolecular Coarse-Grained Modeling of Structure and Dynamics

Theses

1987 – Regine Bohacek – Chemistry Department, Rutgers University
1991 – David Bisant – Genetics Program, George Washington University
2001 – Isabelle Soury-Lavergne – Ecole Normale, Paris
2004 – Moon-ki Kim – Johns Hopkins University, School of Engineering

- 2005 – Haitao Cheng -M.S., Computer Science, ISU
2006 – Peter Vedell – Ph.D., Mathematics and Bioinformatics and Computational Biology, ISU
2007 – Myron Peto – Ph.D., Bioinformatics and Computational Biology, ISU
2007 – Lei Yang – Ph.D., Bioinformatics and Computational Biology, ISU
2008 – Aimin Yan – Ph.D., Bioinformatics and Computational Biology, ISU
2008 – Yaping Feng – Ph.D., Biochemistry, Biophysics and Molecular Biology, ISU
2009 – Haitao Cheng – Ph.D., Bioinformatics and Computational Biology, ISU
2011 – Saraswathi Sundararajan – Ph.D., Bioinformatics and Computational Biology, ISU
2011 – Sumudu Leelananda – Ph.D., Bioinformatics and Computational Biology, ISU
2011 – Michael Zimmermann – Ph.D., Bioinformatics and Computational Biology, ISU
2013 – Ataur Katebi – Ph.D., Bioinformatics and Computational Biology, ISU
2013 – Scott Boyken – Ph.D., Bioinformatics and Computational Biology, ISU
2013 – Yuanyuan Huang – Ph.D., Bioinformatics and Computational Biology, ISU
2016 – Nikita Chopra – Ph.D., Biochemistry, Biophysics and Molecular Biology, ISU
2016 - Kannan Sankar – Ph.D., Bioinformatics and Computational Biology, ISU
2016 – Jie Liu – Ph.D., Bioinformatics and Computational Biology, ISU
2018 – Sambit Mishra – Ph.D., Bioinformatics and Computational Biology, ISU
2018 – Kejue Jia – Ph.D., Bioinformatics and Computational Biology, ISU
2019 – Yuan Wang – Ph.D., Bioinformatics and Computational Biology, ISU
2021 – Sayane Shom – Ph.D., Bioinformatics and Computational Biology, ISU
2022 – Pranav Khade – Ph.D., Bioinformatics and Computational Biology, ISU
2022 – Ambuj Kumar – Ph.D., Bioinformatics and Computational Biology, ISU
2023 – Daniel Kool – Ph.D., Bioinformatics and Computational Biology, ISU

**Presentations and
Invited Participations**

- 2004 – Invited Speaker, Center for Computational Biology, Washington University
2004 – Invited Speaker, Biomedicine Lecture Series, Des Moines University
2004 – Invited Speaker – “Frontiers in Chemistry”, Case Western Reserve University
2004 – Invited Speaker – “Interplay between Computer Modeling and Experiments on Complex Biological Systems”, American Chemical Society, Anaheim
2004 – Invited Speaker – Department of Biochemistry, Georgetown University Medical School
2005 – Invited Speaker – Center for Bioinformatics and Computational Biology, University of Iowa State University
2005 – Invited Speaker – Midwest Computational Structural Biology Workshop
2005 – Invited Speaker – International Center for Theoretical Physics, Trieste, Italy
2005 – Invited Speaker – Center for Bioinformatics and Computational Biology, College of Engineering, University of Iowa
2005 – Invited Speaker – Modeling of Protein Interactions in Genomes, Lawrence, KS
2005 – Invited Speaker – International Meeting on Relaxations in Complex Systems, Lille, France

- 2005 – Invited Speaker – Computational Biology Symposium – National Cancer Institute, Frederick MD
- 2005 – Invited Speaker – Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling: Bridging the Gap, Symposium, American Chemical Society, Washington, DC
- 2005 – Invited Speaker – Multiscale Workshop, Snowbird, UT
- 2005 – Invited Speaker – Department of Electrical and Computer Engineering, ISU
- 2005 – Invited Speaker – NIGMS, NIH, Bethesda
- 2006 – Invited Speaker – Biophysical Society, Workshop on Coarse-Grained Methods for Biomolecular Structure and Dynamics, Salt Lake City
- 2006 – Invited Speaker – Department of Chemistry, University of Oregon
- 2006 – Invited Speaker – Workshop on Rigidity, Flexibility, and Motion in Biomolecules, Tempe, AZ
- 2006 – Invited Speaker – Workshop on Nanomechanics of Biomolecules, Ascona, ETH Conference, Switzerland
- 2007 – Invited Speaker – Nebraska Research and Innovation Conference
- 2007 – Invited Speaker – International Congress on Amino Acids and Proteins, Kallithea, Chalkidiki, Greece
- 2007 – Invited Speaker – Symposium on Structural Determination, Refinement and Modeling of Large Biomolecular Complexes (ACS Meeting, Boston)
- 2007 – Invited Speaker – Centenary Workshop on Multiscale Modeling in Biomolecular Systems, Imperial College, London
- 2007 – Invited Speaker – Indo-US Workshop on Spatial Kinematics and Protein Conformation, Bangalore
- 2008 – Invited Speaker – Protein Folding Symposium, Institute for Mathematics and Its Applications, University of Minnesota
- 2008 – Invited Speaker – Symposium – Multiscale Methods in Biophysics, American Chemical Society, New Orleans
- 2008 – Invited Speaker – Characterizing the landscape: from biomolecules to cellular networks, Telluride
- 2008 – Invited Speaker – Protein Structure & Mechanics, Shanghai
- 2008 – Forefronts of Genomics, University of California, Davis
- 2008 – Invited Speaker – Multiscale Modeling in Soft and Biological Matter, University of Minnesota
- 2009 – Invited Speaker – Structural Biology Department, Hauptman Woodward Medical Research Institute and Roswell Park Cancer Center
- 2009 – Invited Speaker – Conference on Multiscale Soft Matter, Groningen
- 2009 – Invited Speaker – CECAM – Coarse-Graining Biological Systems: Towards Large-Scale Interactions and Assembly, Lausanne
- 2009 – Invited Speaker – BioMAP, Rutgers University
- 2009 – Invited Speaker – Laufer Center for Computational Biology and Genome Sciences, Stony Brook University
- 2009 – Invited Speaker – Biological Sciences, Columbia University
- 2009 – Invited Speaker – Algorithms in Macromolecular Modeling Conference, University of Texas, Austin
- 2010 – Invited Speaker – Distinguished Speaker, University of Pittsburgh
- 2010 – Invited Speaker – Department of Chemistry, Pennsylvania State University
- 2010 – Invited Speaker – Physics Department, Iowa State University
- 2010 – Invited Speaker – Department of Chemistry, University of Cincinnati
- 2010 – Invited Speaker – Department of Chemistry and Physics, University of Missouri
- 2010 – Invited Speaker – NIH Workshop on Enabling Technologies for Structure & Function

- 2010 – Invited Speaker – NIH-NSF Frontiers in Mathematical Biology, University of Maryland
- 2010 – Invited Speaker – RNA in Motion Conference, Iowa State University
- 2010 – Invited Speaker – Modeling of Protein Interactions Meeting, University of Kansas
- 2010 – Invited Speaker – Genetics, Development and Cell Biology Department, Iowa State University
- 2011 – Invited Speaker – Biochemistry Colloquium, University of Wisconsin
- 2011 – Invited Speaker – International Conference on Mathematical Biology, Bangalore
- 2011 – Invited Speaker – Conference on Analysis and Simulation of Biomolecular Structures, Bangalore
- 2011 – Invited Speaker – Telluride Science Research Center – Modeling Biomolecular Structures, Interactions and Functions
- 2011 – American Chemical Society Symposium Denver – Predicting and Disrupting Protein Interactions
- 2011 – Symposium Honoring Harold Scheraga on his 90th Birthday – Cornell University
- 2011 – Physics Department Colloquium – University of Buffalo
- 2011 – Invited Speaker and Organizer – Zing Conference – Protein and RNA Structure Predictions, Mexico
- 2012 – Invited Speaker – Telluride Science Research Center – Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules
- 2012 – Invited Speaker – Department of Biology, University of North Texas
- 2012 – Invited Speaker – Arkansas Bioscience Institute, Arkansas State University
- 2012 – Invited Speaker – Center for Biological Physics, Arizona State University
- 2012 – Invited Speaker – Modeling of Protein Interactions Conference, University of Kansas
- 2012 – Invited Speaker – Morgridge Institute, University of Wisconsin
- 2012 – Invited Speaker – Zing Conference on Mathematical Medicine
- 2013 – Invited Speaker – University of California, Irvine
- 2013 – Invited Speaker – Dynamics Conference, Durham University, UK
- 2013 – Invited Speaker, University of Arkansas, Protein Bioinformatics
- 2013 – Invited Speaker, Biology and Biochemistry Department, University of Houston
- 2013 – Invited Speaker, Modeling Biomolecular Structures, Interactions and Functions, Telluride
- 2013 – Invited Speaker, “Rise of the Machines” on Complex Molecular Systems, Telluride
- 2013 – Invited Speaker, Nationwide Children’s Hospital, Ohio State University
- 2013 – Invited Speaker, 18th Conversation on Biomolecular Structure and Dynamics, Albany
- 2013 – Invited Speaker, Symposium on Coarse-grained Structures, American Chemical Society National Meeting, Indianapolis
- 2013 – Invited Speaker, Zing Mathematical and Computational Medicine, Cancun
- 2014 – Invited Speaker, Challenges in RNA Structural Modeling and Design, Telluride
- 2014 – Invited Speaker, Modeling of Biomolecular Systems Dynamics, Allostery and Regulation: Bridging Experiments and Computations, Istanbul
- 2014 – Invited Speaker, Significance of Knotted Structures for Function of Proteins and Nucleic Acids, Warsaw

- 2014 – Invited Speaker, Department of Computational Medicine and Bioinformatics, University of Michigan Medical School
- 2014 – Invited Speaker, Raymond and Beverly Sackler Institute for Biological, Physical and Engineering Sciences, Yale University
- 2014 – Invited Speaker, Protein Folding, Punta Cana
- 2014 – Chair/Discussion Leader, Biopolymers Gordon Research Conference
- 2014 – Invited Speaker, Modeling of Protein Interactions, University of Kansas
- 2014 – Invited Speaker, Symposium – 40 Years of Protein Structure Analysis, NIH
- 2016 – Invited Speaker, Modeling of Protein Interactions, University of Kansas
- 2017 – Invited Speaker, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University “Protein Structures, Sequences and Mutants”
- 2017 – Invited Speaker, Symposium - Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling,” American Chemical Society, San Francisco
- 2017 – Invited Speaker, University of Texas, Molecular Biophysics Portfolio Program
- 2017 – Invited Speaker, Biochemistry Department, University of California, Riverside
- 2017 – Invited Speaker, Workshop on Deciphering Complex Energy Landscape and Kinetic Network from Single Molecules to Cells, Dijon, France
- 2018 – Invited Speaker, Symposium on Statistical Physics in Biology, Arizona State University
- 2018 – Invited Distinguished Speaker, Computational and Systems Biology, School of Medicine, University of Pittsburgh
- 2018 – Invited Speaker, Modeling of Protein Interactions, University of Kansas
- 2019 – Plenary Speaker, Modeling and Understanding of Structure and Dynamics of Biomolecules, Banff International Research Station for Innovation and Discovery
- 2019 – Invited Speaker, Statistical Mechanics of Chain Molecules, American Chemical Society, San Diego
- 2019 – Invited Speaker, International Conference on Mathematical Multiscale Modeling in Biology, Guanacaste, Costa Rica
- 2022 – Keynote Speaker, International Society for Computational Biology, Madison, WI
- 2022 - Organizer and Speaker, Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride
- 2023 – SHIP Lecutre, Dept Chemistry, University of New Mexico

Reviews

- NIH Special “Roadmap” Study Section for National Centers for Biomedical Computing, ZRG1 BST-C, 2004
- BST-C Study Section Special Emphasis Panel on Cryo-electron microscopy, 2004
- NSF Science and Technology Center, UC Davis, Site Visit, 2004
- NIH Ruth L. Kirschstein National Research Service Application Study Section, 2004
- NIH Computational Biophysics Study Section, 2004
- Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, 2004
- World Bank Panel on Biodiversity, 2004
- Nebraska Research Initiatives, 2004

Texas A&M Research Initiatives, 2005
NIH Special Study Section, 2005
Genome Research Review Committee (NHGRI), 2005
The Wellcome Trust (Joint Infrastructure Fund, UK), 2005
NIH Biophysical and Chemical Sciences Review Group, 2005
NIH Program Project Special Study Section, 2005
DOE Early Career Principal Investigator Program, 2006
NSF Bioinformatics Postdoctoral Panel, 2006
NIH Special Study Section ZRG1 BCMB-B, 2006
Chair, NSF Frontiers in Physics Center and Large ITR Site Visit, 2006
NIH Study Section ZRG1 BCMB-B Biological Chemistry and
Macromolecular Biophysics, 2007
NSF Panel Physics Frontier Centers, 2007, 2008
NSF Bioinformatics Postdoctoral Panel, 2007, 2008, 2009
NIH AED Review Panels, 2007, 2008, 2009
NSF TeraGrid Review Panel, 2009
NIH Challenge Grant Reviews, 2009
NIH Musculoskeletal, Oral and Skin Sciences Review Group, 2009
NIH Special Emphasis Panel BCMB-B, 2009
Defense Threat Reduction Agency, 2009, 2010
Chair, NAS Review Panel on Supercomputing, ANTON, 2010
NIH Special Emphasis Panel on New Biomedical Frontiers at the Interface of
Life and Physical Sciences, 2010
NIH Molecular Structure and Function D, 2011
NSF Site Visit Physics Frontier Center, 2011
Chair, NAS Review Panel on Supercomputing, ANTON, 2011
NIH IAR Study Section, 2011
NIBIB Training Grant Study Section, 2011
NIH-NSF Study Section on Interface between Life and Physical Sciences,
2011
NIH Intramural Review Team – NCI, Laboratory of Molecular Biology, 2011
Institut National du Cancer, mesothelioma review, France, 2011, 2012
NIH Single Molecule Study Section Spring 2012
NIH MSFD Study Section 2012, Spring and Fall
NIH Training Grant Study Section, Fall 2012
Institut National du Cancer, France, grant reviews, 2011, 2012
NSF Science and Technology Center Site Visit, Buffalo, Fall 2012
NIH 2013/05 ZRG1 MOSS-C (56) R RFA RM12-016: NIH Director's New
Innovator Award Study Section 2013
NIH Mid-Point Evaluation of Protein Structure Initiative: Biology Program,
2013
NIH 2013/05 ZRG1 BCMB-B (02) M Biological Chemistry and
Macromolecular Biophysics Study Section, 2013
Chair, NSF Site Visit, Center for Theoretical Biological Physics – Physics
Frontier Center, Rice University, 2013
AAAS Review Panel, South Dakota, 2013
NSF Panel – Physics Frontier Center Pre-Applications, 2013
NSF Physics Frontier Center Site Visit, 2013
NIH Director's New Innovator Reviews, Spring 2014
NIH Big Data to Knowledge Reviews, 2014
NAS Board on Life Sciences, review coordinator Allocation of
Supercomputing Time for the Study of Molecular Dynamics (ANTON),
2014
NIH ZRG1 BST-F 30 I, PAR 14-073 Shared Instrumentation: Bioengineering
Sciences, 2014
NIH-NIBIB Training Grant Reviews, 2014

NIH – Director’s New Innovator Award Reviews, Fall 2014
NIH – New Innovator Grant Reviews, Winter 2015
NIH – Big Data Grant Reviews – Summer 2015
NIH – Molecular Structure and Function – D, Fall 2015
NIH – NIBIB Training Grant Reviews – Fall 2015
NIH – NIH Director’s New Innovator Awards ZRG1-MKOSS-C56 DP2 –
Spring 2016
NSF – Math Bio Cellular Panel – Spring 2016
UC, Irvine – Review of Institute for Genomics and Bioinformatics
NSF- STC Site Visit Center for the Study of Biology with X-Ray Free Electron
Lasers – Summer 2016
NIH – Special Emphasis Panel – Biomedical Research Shared Instrumentation
Grant Reviews, 2016
NAS - ANTON Super-computing awards – Oversight and Coordination,
2016, 2017, 2018, 2019, 2020
NSF – STC Site Visit BioXFEL – Center for the Study of Biology with X-Ray
Free Electron Lasers – May 2017
NIH Chair of Study Section ZRG1 BST-R (30), October 2017
NIH MSFD Study Section February 2018
NSF - CHEM CLP Computational Theory and Modeling Panel April 2018
NSF-PHYS Site Visit Physics Frontier Center for the Physics of Living Cells
– Spring 2019
NIH – NIBIB Training Grant Reviews –2015, 2016, 2017, 2018, 2019 & 2020
NIH Director’s New Innovator Reviews, 2016, 2017, 2018, 2019, 2020, 2021,
2022, 2023

Other Grant Reviews: Israel Science Foundation, NIH Fogarty Scholar-in-Residence Program, DOE, NSF Supercomputer Centers, Review of NRC Review, Advanced Scientific Computing Laboratory – FCRDC, NSF Multidisciplinary Research Review Panel, Packard Foundation, Guggenheim Foundation, Petroleum Research Fund, International Science Foundation, NIH Computational Science and Engineering Program Review and many, many others

Student Selection, Faculty Tenure and Promotion, and Search Committees: Pioneer Fellowship Committee – Iowa State University, many NIH committees, Cornell Univ., Boston University, physics search – Iowa State University, Chief Information and Technology Officer search – Iowa State University, Biomath search at ISU, Faculty Search for Computational Biology (Depts. Math, Stat, CompSci, Comp Eng, ISU) and numerous academic promotion and tenure reviews, BBMB Teaching Evaluation Committee

Center Management

Organized Seminar Series with Many Outside Speakers
Computational Molecular Biology Research Group
Discussion Groups Organized:
Systems Biology Research Group
NextGen Sequencing Research Group
ENCODE Discussion Group
Biological Imaging Research Group
Organized Research Grant Applications and Training Grant Applications
Mentored Young Faculty – helped Assistant Professor (Computer Science)
obtain NSF Career Award upon first application
Provided cost-sharing to strengthen grant applications
Supervised bioinformatics support team
Assisted in development of training grant applications

- Assisted users with hardware and software
- Organized annual research fair
- Organized retreats
- Provided support for graduate students and postdoctoral fellows
- Provided support for student travel
- Supported ISU symposia
- Supported faculty web sites
- Supported Summer Institute in Computational and Systems Biology
- Initiated High Performance Computing Purchase, Installation, and Operations
- Supported servers to distribute software and provide access to software

Present Funding

- NSF-MCB Defining the Architecture of the Pyk2 Activation Complex (PI: Underbakke)
- NSF-MCB Defining the Structural Organization of the Polysaccharide-Synthesizing Complexes Localized in Golgi (PI: Zobotina)
- NIH-HGRI R01 Novel Use of Genome Information to Understand Mutations (PI)
- NIH-NIGMS R01 Statistics of Sequence Correlations for Reliable Inferences (Co-PI)
- DOE Novel Systems Approach for Rational Engineering of Robust Microbial Metabolic Pathways (Co-PI)
- USDA Development and utilization of genomic and genomic approaches to efficiently exploit genetic variation for crop improvement (Co-PD)

Planned Research

- Identifying in-depth functions of genes/proteins
- Improved Gene Annotations from New Protein Function Identifications
- Using Large Protein Language Model Embeddings as Data
- Cross-species comparisons of gene networks for cancer genes
- Networks to connect broadly across space, time and species
- P53 mutants and restoring function by identifying compensating mutations in other genome
- Compensating mutations that restore functional dynamics
- Conformational entropies and disordered proteins
- Novel Use of Genome Information to Understand Mutations
- New Structure-Based Phylogenies of Genes and Proteins
- Employing Linguistic Models and Machine Learning for Improved Identification of Protein Functions
- Linguistic Models and Biological Complexity