GAREGIN A. PAPOIAN

Department of Chemistry & Biochemistry
Institute for Physical Science and Technology
University of Maryland
College Park, MD 20742-4454
E-mail: gpapoian@umd.edu

APPOINTMENTS

2014-Present	Monroe Martin Professor, Department of Chemistry and Biochemistry & Institute for Physical Science and Technology , University of Maryland	College Park, MD
2014-Present	Director of the Chemical Physics Program at the University of Maryland	College Park, MD
2010-2014	Monroe Martin Associate Professor, Department of Chemistry and Biochemistry & Institute for Physical Science and Technology , University of Maryland	College Park, MD
2004-2010	Assistant Professor, Department of Chemistry, The University of North Carolina at Chapel Hill (tenured in 2010)	Chapel Hill, NC
2001-2004	Department of Chemistry, University of California, San Diego NIH Postdoctoral Research Associate; *Adviser: Prof. P. G. Wolynes*	La Jolla, CA
2000	Department of Chemistry, The University of Pennsylvania Postdoctoral Research Associate; *Adviser: Prof. M. L. Klein*	Philadelphia, PA
1995-1999	Department of Chemistry, Cornell University Graduate Research Assistant; *Ph.D. Adviser: Prof. R. Hoffmann*	Ithaca, NY

EDUCATION

1995-1999	Cornell University, Ph.D.	Ithaca, NY
1990-1994	Russian Academy of Sciences, Higher Chemical College	Moscow, Russia
1990	High School of Physics & Mathematics	Yerevan, Armenia

HONORS AWARDS

2011	• Rice Family Fund Fellowship Award, The Kavli Institute for Theoretical Physics	Santa Barbara, CA
2010-Present	• Faculty of 1000 member	
2010	• Phillip and Ruth Hettleman Prize for Artistic and Scholarly Achievement	Chapel Hill, NC
2010	• ACS Hewlett-Packard Outstanding Junior Faculty Award	USA
2009-2014	• National Science Foundation CAREER Award	USA
2008-2013	• Camille Dreyfus Teacher-Scholar	USA
2007-2010	• Beckman Young Investigator	USA
2004-2009	• Camille and Henry Dreyfus New Faculty Award	USA
2005	• R. J. Reynolds Excellence Junior Faculty Development Award	Chapel Hill, NC
2001-2004	• National Institute of Health Postdoctoral Fellowship	USA
1999	• Wentink Prize to Outstanding Graduate Students, Cornell University	Ithaca, NY
1997-1998	• Wachter Memorial Award for Outstanding Research in Physical Chemistry, Cornell University	Ithaca, NY
1995	• H. P. Cady Award for Academic Excellence, The University of Kansas	Lawrence, KS

1992	• Mendeleev Award for Outstanding Undergraduate Student Research in Russia
1988-1990	• Winner of National Olympiads among high school students in the Republic of Armenia and USSR (Biology, Chemistry, Mathematics and Physics)

Publication List

h-index (Feb 2016):
Google Scholar: 28; Total Citations: 2340
Web of Science: 25; Total Citations: 1911
⋆ indicates that G. A. Papoian was either the corresponding author or among the corresponding authors

UMD

2016

71. B. Zhang, W. Zheng, G. A. Papoian, and P. G. Wolynes, "Exploring the Free Energy Landscape of Nucleosomes", **J Am Chem Soc**, (2016), submitted

⋆70. K. Popov, J. Komianos, G. A. Papoian "MEDYAN: Mechanochemical Simulations of Actomyosin Networks and Other Active Matter", **PLOS Comp Bio**, (2016), submitted

⋆69. U. Dobramysl, G. A. Papoian, and R. Erban "Steric Effects Induce Geometric Remodeling of Actin Bundles in Filopodia", **Biophys J**, (2016), in press

⋆68. A. Davtyan, M. Platkov, M. Gruebele, G. A. Papoian, 'Stochastic Resonance in Protein Folding Dynamics", **ChemPhysChem**, (2016), in press

⋆67. K. Dave, A. Davtyan, G. A. Papoian, M. Gruebele, M. Platkov 'Environmental Fluctuations and Stochastic Resonance in Protein Folding", **ChemPhysChem**, (2016), DOI: 10.1002/cphc.201501041

2015

⋆66. D. Winogradoff, H. Zhao, Y. Dalal, G. A. Papoian, "Shearing of the CENP-A dimerization interface mediates plasticity in the octameric centromeric nucleosome", **Sci Rep**, (2015), 5, 17038, DOI: 10.1038/srep17038

⋆65. D. Winogradoff, I. Echeverria, D. A. Potoyan, G A. Papoian "The acetylation landscape of the H4 histone tail: disentangling the interplay between the specific and cumulative effects", **J Am Chem Soc**, (2015), 137 (19), 6245-6253

⋆64. I. Echeverria, G. A. Papoian "DNA Exit Ramps Are Revealed in the Binding Landscapes Obtained from Simulations in Helical Coordinates", **PLOS Comp Bio**, (2015), DOI: 10.1371/journal.pcbi.1003980

2014

⋆63. I. Echeverria, D. E. Makarov, G. A. Papoian "Concerted Dihedral Rotations Give Rise to Internal Friction in Unfolded Proteins", **J Am Chem Soc**, (2014), 136 (24), 8708-8713

⋆62. I. Echeverria, G. A. Papoian "Structural Heterogeneity and Dynamics of the Unfolded Ensemble", **Israel J Chem**, (2014), 54 (8-9), 1293-1301

⋆61. R. Erban, M. B. Flegg, G. A. Papoian "Multiscale Stochastic Reaction-Diffusion Modelling: Application to Actin Dynamics in Filopodia", **Bull of Mat Biol**, (2014), 2014, 76, 799-818

2013

⋆60. K. Popov and G. A. Papoian "Capsid Deformations Reveal Complex Mechano-Chemistry", **Biophysical Journal**, (2013), 105 (10), 2233-2234

⋆59. L. Hu and G. A. Papoian "Molecular Transport Modulates the Adaptive Response of Branched Actin Networks to an External Force", **J Chem Phys B**, (2013), 117 (42), 13388-13396

⋆58. D. Ma, S. E. Bettis, K. Hanson, M. Minakova, L. Alibabaei, W. Fon-drie, D. M. Ryan, G. A. Papoian, T. J. Meyer, M. L. Waters, and J. M. Papanikolas "Interfacial Energy Conversion in Ru(II) Polypyridyl-Derivatized Oligoproline Assemblies on TiO2 ", **J Am Chem Soc**, (2013), 135, 5250-5253

⋆57. D. Potoyan, A. Savelyev, G. A. Papoian "Recent Successes in Coarse Grained Modeling of DNA", **WIREs Computational Molecular Science**, (2013), 3, 69-83

2012

56. W. Zheng, N. P. Schafer, A. Davtyan, G. A. Papoian, P. G. Wolynes "Predictive Energy Landscapes for Protein-Protein Association", **Proc Nat Acad Sci USA**, (2012), 109, 19244-19429

⋆55. D. Potoyan and G. A. Papoian "The Regulation of the H4 Tail Binding and Folding Landscapes via Lys-16 Acetylation", **Proc Nat Acad Sci USA**, (2012), 109, 17857-17862

⋆54. P. I. Zhuravlev, Y. Lan, M. S. Minakova, and G. A. Papoian "Theory of Active Transport in Filopodia and Stereocilia", **Proc Natl Acad Sci USA**, (2012), 109, 10849-10854

⋆53. M. Rubinstein and G. A. Papoian "Polyelectrolytes in Biology and Soft Matter", **Soft Matter**, (2012), 8, 9265-9267

⋆52. A. Davtyan, W. Zheng, N. Schafer, C. Clementi, P. G. Wolynes and G. A. Papoian "AWSEM-MD: Protein Structure Prediction Using Coarse-grained Physical Potentials and Bioinformatically Based Local Structure Biasing", **J Phys Chem B**, (2012), 116, 8494-8503

⋆51. D. J. Wilger, S. Bettis, C. K. Materese, M. Minakova, G. A. Papoian, J. M. Papanikolas, M. L. Waters "Position-Dependent Energy Transfer between Ruthenium(II) and Osmium(II) Modified Coiled-Coil alpha-Helical Peptide Dimers", **Inorg Chem**, (2012), 51, 11324-11338

⋆50. D. Potoyan and P. I. Zhuravlev and G. A. Papoian "Computing Free Energy of a Large-Scale Allosteric Transition in Adenylate Kinase (ADK) using All Atom Explicit Solvent Simulations", **J Phys Chem B**, (2012), 116, 1709-1715

⋆49. P. I. Zhuravlev, L. Hu, and G. A. Papoian "Computer Simulations of Mechano-Chemical Networks Choreographing Actin Dynamics in Cell Motility", **Contributed Book Chapter in "Computational Modeling of Biological Systems: From Molecules to Pathways", Publisher: Springer, edited by N. Dokholyan**, (2012), ISBN-10: 1461421454

2011

⋆48. A. Savelyev, C. K. Materese, and G. A. Papoian "Is DNAs Rigidity Dominated by Electrostatic or Nonelectrostatic Interactions?", **J Am Chem Soc**, (2011), 133, 19290-19293

⋆47. P. I. Zhuravlev and G. A. Papoian "Protein Fluxes Along the Filopodium As a Framework for Understanding the Growth-Retraction Dynamics: the Interplay Between Diffusion and Active Transport", **Cell Adhes & Migr (Special Issue on Filopodia)**, (2011), 5, 448-456

⋆46. L. Hu and G. A. Papoian "How does the Antagonism Between Capping and Anti-Capping Proteins Control Actin Network Dynamics?", **Journal of Physics: Condensed Matter (Special Issue on "Cooperative dynamics in cells")**, (2011), 23, 374101

⋆45. M. Minakova, A. Savelyev and G. A. Papoian "Non-equilibrium Water Transport in a Nonionic Microemulsion System", **J Phys Chem B**, (2011), 115, 6503-6508

⋆44 D. Potoyan and G. A. Papoian "Energy Landscape Analyses of Disordered Histone Tails Reveal Special Organization of Their Conformational Dynamics", **J Am Chem Soc**, (2011), 133, 7405-7415

2010

⋆43. P. I. Zhuravlev, and G. A. Papoian "Protein Functional Landscapes, Dynamics, Allostery: A Tortuous Path Towards a Universal Theoretical Framework", **Quater Rev Biophys**, (2010), 43, 295-332

UNC

⋆42. A. Savelyev and G. A. Papoian "Chemically Accurate Coarse-Graining of Double-Stranded DNA", **Proc Natl Acad Sci USA**, (2010), 107, 20340

41. V. Oklejas, C. Zong, G. A. Papoian, P. G. Wolynes "Protein Structure Prediction: Do Hydrogen Bonding and Water-Mediated Interactions Suffice?", **Methods**, (2010), 52, 84-90

⋆40. P. I. Zhuravlev, S. Wu, D. Potoyan, M. Rubinstein and G. A. Papoian "Computing Free Energies of Protein Conformations from Explicit Solvent Simulations", **Methods**, (2010), 52, 115-121

⋆39. P. I. Zhuravlev, B. Der and G. A. Papoian "Design of Active Transport Must Be Highly Intricate: a Possible Role of Myosin and Ena/Vasp for G-Actin Transport in Filopodia", **Biophys J**, (2010), 98, 1439-1448

⋆38. L. Hu and G. A. Papoian "Mechano-Chemical Feedbacks Regulate Actin Mesh Growth in Lamellipodial Protrusions", **Biophys J**, (2010), 98, 1375-1384

⋆37. N. Tanaka and G. A. Papoian "Reverse-Engineering of Biochemical Reaction Networks from Spatio-Temporal Correlations of Fluorescence Fluctuations", **J Theor Biol**, (2010), 264, 490500

⋆36. P. I. Zhuravlev, and G. A. Papoian "Functional vs. Folding Landscapes: The Same yet Different", **Curr Opin Struct Biol**, (2010), 20, 16-20

2009

⋆35. C. K. Materese, A. Savelyev, and G. A. Papoian "Counterion Atmosphere and Hydration Patterns near a Nucleosome Core Particle ", **J Am Chem Soc**, (2009), 131, 1500515013

⋆34. P. I. Zhuravlev and G. A. Papoian "Molecular Noise of Capping Protein Binding Induces Macroscopic Instability in Filopodial Dynamics", **Proc Natl Acad Sci USA**, (2009), 106, 11570-11575

⋆33. P. I. Zhuravlev, C. K. Materese and G. A. Papoian "Deconstructing the Native State: Energy Landscapes, Function and Dynamics of Globular Proteins", **J Phys Chem B (Feature Article, July 2 2009 Journal Cover)**, (2009), 133, 8800-8812

⋆32. A. Savelyev and G. A. Papoian "Molecular Renormalization Group Coarse-Graining of Electrolyte Solutions: Application to Aqueous NaCl and KCl", **J Phys Chem B**, (2009), 133, 7785-7793

⋆31. A. Savelyev and G. A. Papoian "Molecular Renormalization Group Coarse-Graining of Polymer Chains: Application to Double-Stranded DNA", **Biophys J**, (2009), 96, 4044-4052

2008

⋆30. Y. Lan, T. C. Elston, and G. A. Papoian "Elimination of Fast Variables in Chemical Langevin Equations", **J Chem Phys**, (2008), 129, 214115

⋆29. S. Wu, P. I. Zhuravlev and G. A. Papoian "High Resolution Approach to the Native State Ensemble Kinetics and Thermodynamics", **Biophys J**, (2008), 95, 5524-5532

⋆28. G. A. Papoian "Proteins with weakly funneled energy landscapes challenge the classical structure-function paradigm", **Proc Natl Acad Sci USA**, (2008), 105, 14237-14238

⋆27. C. K. Materese, C. C. Goldmon and G. A. Papoian "Hierarchical Organization of Eglin C Native State Dynamics Is Shaped by Competing Direct and Water-Mediated Interactions", **Proc Natl Acad Sci USA**, (2008), 105, 10659-10664

⋆26. A. Savelyev and G. A. Papoian "Polyionic Charge Density Plays a Key Role in Differential Recognition of Mobile Ions by Biopolymers", **J Phys Chem B**, (2008), 112, 9135-9145

⋆25. Y. Lan and G. A. Papoian "The Stochastic Dynamics of Filopodial Growth", **Biophys J**, (2008), 94, 3839-3852

2007

⋆24. Y. Lan and G. A. Papoian "Stochastic resonant signaling in enzyme cascades", **Phys Rev Lett**, (2007), 98, 228301

⋆23. A. Savelyev and G. A. Papoian "Inter-DNA Electrostatics from Explicit Solvent Molecular Dynamics Simulations", **J Am Chem Soc**, (2007), 129, 6060-6061

⋆22. Y. Lan and G. A. Papoian "Evolution of Complex Probability Distributions in Enzyme Cascades", **J Theor Biol**, (2007), 248, 537-545

⋆21. A. Savelyev and G. A. Papoian "Free energy calculations of Na^+ and K^+ partitioning between DNA and chloride solutions ", **Mend Comm**, (2007), 17, 97-99

20. J. Lätzer, G. A. Papoian, M. C. Prentiss, E. A. Komives, and P. G. Wolynes "Induced Fit, Folding, and Recognition of the NF-κB-Nuclear Localization Signals by IκBα and IκBβ", **J Mol Biol**, (2007), 367, 262-274

2006

⋆19. A. Savelyev and G. A. Papoian "Electrostatic, steric, and hydration interactions favor Na^+ condensation around DNA compared with K^+", **J Am Chem Soc**, (2006), 128, 14506-14518

⋆18. Y. Lan, P. G. Wolynes, and G. A. Papoian "A variational approach to the stochastic aspects of cellular signal transduction", **J Chem Phys**, (2006), 125, 124106

⋆17. Y. Lan and G. A. Papoian "The interplay of discrete noise and nonlinear chemical kinetics in a signal transduction cascade", **J Chem Phys**, (2006), 125, 154901

UCSD

16. C. Zong, G. A. Papoian, J. Ulander, and P. G. Wolynes "The Role of Topology, Nonadditivity and Water Mediated Interactions in Predicting the Structures of α/β Proteins", **J Am Chem Soc**, (2006), 128, 5168-5176

2004

15. G. A. Papoian, J. Ulander, M. E. Eastwood, Z. Luthey-Schulten, and P. G. Wolynes "Water in Protein Structure Prediction", **Proc Natl Acad Sci USA**, (2004), 101, 3352-3357.

14. Y. Levy, G. A. Papoian, J. N. Onuchic, and P. G. Wolynes "The Energy Landscape Analysis of Protein Dimers", **Israel J Chem**, (2004), 44, 281-297.

13. G. A. Papoian, J. Ulander, and P. G. Wolynes "The Role of Water Mediated Interactions in Protein-Protein Recognition Landscapes.", **J Am Chem Soc**, (2003), 125, 9170-9178,

2003

12. G. A. Papoian and P. G. Wolynes "The Physics and Bioinformatics of Binding and Folding — an Energy Landscape Perspective" **Biopolymers**, (2003), 68, 333-349,

UPenn

11. G. A. Papoian, W. F. DeGrado, and M. L. Klein "Probing the Configurational Space of a Metalloprotein Core: An *ab Initio* Molecular Dynamics Study of Duo Ferro 1 binuclear Zn Cofactor." **J Am Chem Soc**, (2003), 125, 560-569,

Cornell

2001

10. G. A. Papoian and R. Hoffmann "Electron-rich Rods as Building Blocks for Sb Strips and Te sheets"; **J Am Chem Soc**, (2001), 123, 6600-6608,

9. A. Ienco, R. Hoffmann, and G. A. Papoian "Electron-rich bonding and the Importance of s,p mixing as One Moves Across a Period: A Lesson from the LiSn System." **J Am Chem Soc**, (2001), 123, 2317-2325,

2000

8. G. A. Papoian and R. Hoffmann "Hypervalent Bonding in One, Two and Three Dimensions: Extending the Zintl-Klemm Concept to Nonclassical Electron-Rich Networks." **Angew Chem**, (2000), 39, 2408-2448,

7. G. A. Papoian, J. K. Nørskov, and R. Hoffmann "A comparative study of hydrogen, methyl, and ethyl chemisorption on the Pt (111) surface." **J Am Chem Soc**, (2000), 122, 4129-4144,

6. D. -K. Seo, G. A. Papoian, and R. Hoffmann. "Generalized Perturbational Molecular Orbital (PMO) Theory" **Int J Quant Chem**, (2000), 77, 408-420

1999

5. W. V. Glassey, G. A. Papoian, and R. Hoffmann "Total energy partitioning within an extended Hückel framework: a Hamilton Population study of surface — CO interaction in the c(2x2) — CO/Ni(100) chemisorption system" **J Chem Phys**, (1999), 111, 893-910,

1998

4. G. A. Papoian and R. Hoffmann " Building up complexity from strips and sheets — the electronic structure of the $La_{12}Mn_2Sb_{30}$ alloy" **J Solid State Chem**, (1998), 139, 8-21,

3. G. A. Papoian, K.P. Butin, R. Hoffmann, and V.I Rozenberg "Theoretical investigation of [2.2]paracyclophane as a donor toward $Cr(CO)_3$ group" **Russ Chem Bull**, (1998), 47, 153-159

U. Kansas

1996

2. G. A. Papoian, K. Gu, J. Wiorkiewicz-Kuczera, K. Kuczera, and K. Bowman-James. "Molecular dynamics simulations of nitrate complexes with polyammonium macrocycles: insight on phosphoryl transfer catalysis." **J Am Chem Soc**. (1996), 118, 1354-64,

Russia

1993

1. S. Nefedov, A. Pasynskii, I. Eremenko, G. A. Papoian, L. Rubinstein, A. Yanovskii, and Yu. Struchkov. "Electron control of metal-metal bond multiplicity in binuclear thiolate-bridged rhenium-molybdenum complexes". **Russ J Inorg Chem**, (1993) , 38, 69-7,

PROFESSIONAL SERVICE

Editorial Board Member	
2012-Present	**F1000 Research**, Editorial Board Member
2011-Present	**BMC Biophysics**, Section Editor & Editorial Board Member
Manuscript Reviewer	Acc. Chem. Res., Biochemistry, Biophys J, Biopolymers, Canad. J. Chem., Chem. Phys. Lett., EMBO Reports, J Am Chem Soc, J Chem Phys, J. Mol. Model., J Phys Chem, J. Struct. Biol., J. Theor. Biol., Mol. Sim., Proteins, Soft Matter, Structure, PLOS Comp. Biol., Proc Natl Acad Sci USA

Proposal Reviewer	National Science Foundation; National Science Foundation Study Panels; National Institute of Health Panel; Petroleum Research Fund
Departmental Service	Director of Chemical Physics Program (IPST; 2014-present); Chair of the Faculty Advisory Committee (Chemistry and Biochemistry; 2015-2016); Associate Chair of the Department of Chemistry and Biochemistry (2012-2014); Graduate Studies Committee (Chemistry and Biochemistry; *Chair* 2012-2014); Graduate Executive Committee (Chemistry and Biochemistry; 2012-2014); Faculty Advisory Committee (Chemistry and Biochemistry; 2011-2012); Executive Committee (Chemistry and Biochemistry; 2012-2016); Q-Bio Cluster Hire Search Committee (2012-2014)

CONFERENCE ORGANIZER

Mar 18, 2013	American Physical Society National Meeting: A Symposium on "Multiscale modeling: Coarse-graining in space and time"; *Meeting Co-Chair*	Baltimore, MD
Feb 2, 2013	Biophysical Society Meeting: 7th Annual IDP Subgroup Symposium; *Meeting Co-Chair*	Philadelphia, PA
Feb 27, 2012	American Physical Society National Meeting: A Symposium on "Hydrophobic Interactions and Hydrogen Bonding Networks in Polymeric and Soft Matter Systems"; *Meeting Chair*	Boston, MA
August 8, 2010	The Fourth Shanghai International Conference on Biophysics and Molecular Biology; *Meeting Co-Chair*	Shanghai, China
May 17, 2010	An International Symposium on "Solvation and Ionic Effects in Biomolecules: Theory to Experiment"; *Meeting Co-Chair*	Tsakhkadzor, Armenia
Mar 20, 2009	American Physical Society National Meeting: Invited Symposium on Biological Polyelectrolytes; *Meeting Chair*	Pittsburgh, PA
Feb 1-4, 2009	Mesilla Chemistry Workshop on Multi-Scale Modeling of Biological Molecules; *Meeting Co-Chair*	Mesilla, NM

CURRENT FUNDING

National Science Foundation, CHE-1363081
(PI: Papoian)
Mechanochemistry of Actin Networks
06/01/2014-05/31/2017

NCI-UMD Partnership for Cancer Technology
(PIs: Papoian, Dalal))
"High-Resolution Atomistic Simulations and Experimental Characterizations of CENP-A/H3 Hybrid Nucleosomes"
09/02/2015-09/1/2017

COMPLETED FUNDING

National Science Foundation, CHE-1206060
(PI; Upadhyaya; co-PI: Papoian)
"Physical aspects of lymphocyte activation"
09/01/2012-08/31/2015

NCI-UMD Partnership for Cancer Technology
(PIs: Papoian, Dalal))
"Computational Modeling and Experimental Perturbations of the Centromeric Chromatin Fiber"
09/02/2013-09/1/2014

National Science Foundation, CAREER Award, CHE-0846701
(PI: Papoian)
CAREER: Physico-Chemical Modeling of Filopodia Initiation, Dynamics, and Spatio-Temporal Regulation
05/01/2009-04/30/2014

Department of Energy, Energy Frontier Research Centers (EFRC)
(PI: Meyer; CoPI: Papoian)
Solar Fuels and Next Generation Photovoltaics
05/01/2009-04/30/2014

Camille Dreyfus Teacher-Scholar Award, Camille and Henry Dreyfus Foundation
(PI: Papoian)
Multi-Scale Modeling of Biophysical Processes in the Cell
05/2008-04/2013

National Science Foundation, Award, CBET-1032428
(PI: Papoian)
An International Symposium on Solvation and Ionic Effects in Biomolecules: Theory to Experiment
04/20/2010-04/20/2011

Beckman Young Investigator Award
(PI: Papoian)
Electrostatic and structural mechanisms of chromatin folding regulation by histone tail posttranslational modifications
09/01/2007-08/31/2010

Petroleum Research Fund, Award# 47593-G6
(PI: Papoian)
Investigating topological transitions among soft mesoscopic structures in microemulsions with all-atom and coarse-grained simulations
05/01/08-04/30/10

National Science Foundation, Award# CHE-715225
(PI: Papoian)
Mechano-Chemical Approach to Actin Filament Bundle Self-Assembly and Growth
08/15/2007-08/14/2009

New Faculty Award, Camille and Henry Dreyfus Foundation
(PI: Papoian)
Fluctuations and the Physical Chemistry of the Cell
8/1/04-7/31/09

North Carolina Biotechnology Center, Multidisciplinary Research Grant
(PI: Strahl; CoPI: Papoian)
Regulation of Nucleosome Stability as a Mediator of Chromatin Function
04/01/06-03/31/08

Junior Faculty Development Award, The University of North Carolina at Chapel Hill
(PI: Papoian)
Stochastic Theory of Protein Signal Transduction Pathways
01/01/05-12/31/05

TEACHING

Fall 2015	"Chemical and Statistical Thermodynamics"	Chem 684
Fall 2014	"Chemical and Statistical Thermodynamics"	Chem 684
Fall 2013	"Physical Chemistry II: Quantum Chemistry"	Chem 482
Fall 2012	"Physical Chemistry II: Quantum Chemistry"	Chem 482
Spring 2012	"Statistical Mechanics and Chemistry"	Chem 687
Fall 2011	"Physical Chemistry II: Quantum Chemistry"	Chem 482
Spring 2011	"Theory of Soft Matter and Biopolymers"	Chem 699/ChPh 618E
Fall 2009	"Thermodynamics and Introduction to Statistical Thermodynamics"	Chem 484/MTSC 730
Fall 2009	"Macromolecular Structure and Dynamics"	BioC 651
Spring 2009	"Soft Matter Theory"	Chem 786
Fall 2008	"Macromolecular Structure and Dynamics"	BioC 651
Fall 2007	"Thermodynamics and Introduction to Statistical Thermodynamics"	Chem 484/MTSC 730
Fall 2007	"Macromolecular Structure and Dynamics"	BioC 651
Spring 2007	"Soft Matter Theory"	Chem 786
Fall 2006	"Macromolecular Structure and Dynamics"	BioC 651
Spring 2006	"Physical Chemistry I: Thermodynamics"	Chem 481
Fall 2005	"Thermodynamics and Introduction to Statistical Thermodynamics"	Chem 484/MTSC 730
Spring 2005	"Physical Chemistry I: Thermodynamics"	Chem 481

CURRENT GROUP MEMBERS

Graduate Students

2012-Present	*Haiqing Zhao*, Biophysics Program	4^{th} year student
2014-Present	*James Komianos*, Biophysics Program	3^{rd} year student
2014-Present	*Hao Wu*, Biophysics Program	3^{rd} year student
2014-Present	*Mary Pitman*, Chemistry Program	2^{nd} year student
2015-Present	*Aravind Chandrasekaran*, Chemistry Program	2^{nd} year student
2016-Present	*Qin Ni*, Chemical Engineering	1^{st} year student

Undergraduate Students

2015-present	*Robert Liu*, UMD College Park	Senior
2015-present	*Jeffrey Wang*, UMD College Park	Junior

FORMER GROUP MEMBERS

Postdoctoral Associates

2011-2015	*Dr. Ignacia Echeverria*, is currently a postdoctoral research associate with Prof. Andrej Sali at UCSF
2011-2014	*Dr. Konstantin Popov* is currently a Research Assistant Professor at the University of North Carolina in Chapel Hill
2008-2013	*Dr. Longhua Hu* is currently a researcher at the National Institute of Health in Bethesda, MD

2004-2007	*Dr. Yueheng Lan* is currently an Assistant Professor in the Department of Physics at Tsinghua University, Beijing, China	
2005-2007	*Dr. Sangwook Wu* is currently a postdoctoral associate with Professor Lee Pedersen at UNC Chapel Hill	
2005-2010	*Dr. Alexey Savelyev* is currently a research scientist at the Institute of Applied Physics in Sumi, Ukraine	

Graduate Students

2011-2015	*David Winogradoff*, B.S. Haverford College, Thesis Title: "Molecular Dynamic Simulations of Nucleosomes and Histone tails: the Effects of Histone variance and Post-Translational modification"; Currently a postdoctoral fellow with Prof. A. Aksimentiev at the University of Illinois at Urbana-Champaign	Ph.D., 2015
2008-2013	*Aram Davtyan*, B.S. Yerevan State University, Armenia, 2008; Thesis Title: "Computer Simulations of Protein Folding"; Currently a postdoctoral fellow with Prof. G. Voth at the University of Chicago	Ph.D., 2013
2007-2012	*Davit Potoyan*, B.S. Yerevan State University, Armenia, 2006; Thesis Title: "Using Energy Landscape Theory to Uncover the Organization of Conformational Space of Proteins in Their Native States."; Currently a postdoctoral fellow with Prof. P. G. Wolynes at Rice University	Ph.D., 2012
2007-2012	*Maria Minakova*, M.S. Moscow State University, Russia, 2006; Thesis Title: "Advanced Computer Simulations Of Nanomaterials And Stochastic Biological Processes."; Currently a data scientist at Facebook	Ph.D., 2012
2005-2010	*Pavel Zhuravlev*, M.S. Moscow State University, Russia, 2005; Thesis Title: "Unraveling the complexity of biological processes from protein native dynamics to cell motility in molecular simulations."; Currently a postdoctoral fellow with Prof. D. Thirumalai at UMD College Park	Ph.D., 2010
2005-2010	*Christopher Materese*, B.S. Pennsylvania State University, 2005; Thesis Title: "Atomistic simulations uncover microscopic details of nucleosomal electrostatics, energy landscapes of proteins and photovoltaic polymer dynamics."; Currently a postdoctoral fellow at NASA, Ames, CA	Ph.D., 2010
2007-2008	*Natsuki Tanaka*, B.S. Osaka University, 2005; Thesis Title: "Spatio-Temporal Correlation Analysis of Rho activation Dynamics Observed by Fluorescence Microscopy Using Stochastic Simulations "	M.S., 2008

Rotation Students

2012	*John Giannini Jr*, Biohysics Program, UMD College Park	1^{st} year student
2011	*Desu Chen*, Biohysics Program, UMD College Park	1^{st} year student
2011	*Brian Stock*, Biohysics Program, UMD College Park	1^{st} year student
2011	*Yonathan Cwik*, Biophysics Program, UMD College Park	1^{st} year student

2011	*Ruiliang Bai*, Biophysics Program, UMD College Park	1st year student
2009	*Ryan Vary*, Department of Chemistry, UNC Chapel Hill	1st year student
2009	*Bryan Der*, Biophysics Program, UNC Chapel Hill	1st year student
2009	*Elizabeth Proctor*, Biophysics Program, UNC Chapel Hill	1st year student
2009	*Weston Smith*, Biophysics Program, UNC Chapel Hill	1st year student
2008	*Mohona Sarkar*, Department of Chemistry, UNC Chapel Hill	1st year student
2006	*Justin Low*, Biophysics Program, UNC Chapel Hill	1st year student
2005	*Jeremy Deyton*, Department of Chemistry, UNC Chapel Hill	1st year student

Undergraduate Students

2011-2014	*Michelle Thomas (Beckman Scholar)*, UMD College Park	Sophomore
2012-2013	*James Ritchie*, UMD College Park	Senior
2011-2012	*Steven Silverman*, University of Maryland, College Park	Senior
2010-2012	*Michael Polynski*, HPC Russian Academy of Sciences	Junior
2010-2011	*Sean P. Doyle*, UNC Chapel Hill	Senior
2010	*Bryan McPhatter*, UNC Chapel Hill	Junior
Summer 2009	*Gregory Rubinstein*, California Institute of Technology	Junior
Summer 2008	*Maria Colorado*, UC Davis, supported by the Biophysics Summer Course for Minority Students at UNC-CH	Junior
2007-2008	*Michael Pham*,UNC Chapel Hill	Freshman
2007-2008	*Kevin McElligott*, UNC Chapel Hill	Junior
2007-2008	*Giovanni Pulaj*, UNC Chapel Hill	Junior
2005-2006	*Sean Walder*, UNC Chapel Hill	Sophomore

High School Students

2011-2012	*Kate Coppess*, Eleanor Roosevelt High School, Greenbelt, Maryland	Senior
Summer 2007	*Christa Goldmon*, Jordan High School, Durham, North Carolina	Junior
Summer 2007	*Michael Pham*, The North Carolina School of Science and Mathematics, Durham, North Carolina	Senior

INVITED LECTURES

Conferences

Mar 1, 2016	**"Multiscale methods for stochastic dynamical systems in biology"**, "Molecular Simulations of Acto-Myosin Network Dynamics"	Edinburgh, Scotland
Nov 10, 2015	**VI International Symposium on Biochemistry and Molecular Biology**, "Developing a Transferable Coarse-Grained Protein Model and Applying it to the Chromatin Folding Problem"	Havana, Cuba
Sep 14, 2015	**SciCADE 2015 (Scientific Computation And Differential Equations)**, "Accelerating Simulations of Reaction-Diffusion Mechanochemistry in Acto-Myosin Networks"	Potsdam, Germany
Jul 17, 2015	**iPoLS 2015 Annual Meeting**, "Computational Modeling of the Eukaryotic Cytoskeleton"	Arlington, VA

Jun 10, 2015	**ACS NERM**, "The Acetylation Landscape of the H4 Histone Tail"	Ithaca, NY
May 26, 2015	**8th Chaotic Modeling and Simulation International Conference**, "Pattern Formation in Acto-Myosin Networks"	Paris, France
Mar 22, 2015	**ACS National Meeting, Symposium on Progress and Challenges in Molecular Simulations of Biomolecules**, "Atomistic and Coarse-Grained Simulations of Histones, Nuclesomes and DNA"	Denver, CO
Sep 7, 2014	**Mathematics of the Cell**, "Detailed Computational Modeling of the Eukaryotic Cytoskeleton"	Banff, Canada
Jul 21, 2014	**Plenary Talk: American Conference of Theoretical Chemistry (ACTC)**	Telluride, CO
Jul 16, 2014	**Zing Conference on Protein Folding**, "Binding and Folding Landscapes of Ubiquitin and Histone Dimers and Oligomers"	Dominican Republic
Jul 6, 2014	**Enhanced Sampling Techniques in Simulation of Complex Systems within the 10th American Institute of Mathematical Sciences (AIMS) Conference on Dynamical Systems, Differential Equations and Applications**, "Computing Free Energy Landscapes of Small Molecules Interacting with DNA"	Madrid, Spain
Jul 11, 2014	**7th World Congress of Biomechanics**	Boston, MA
Jun 15, 2014	**Coarse-graining as a Frontier of Statistical Mechanics**,	Santa Fe, NM
May 22, 2014	**1st Symposium on Current Topics in Molecular Biophysics**, "Binding and Folding Landscapes of Ubiquitin, Histones and Their Chaperones"	So Paulo, Brazil
Aug 3, 2013	**KITPC Symposium on "Physical Principles and Underlying Mechanisms of Biomolecules and Materials"**, "Understanding the Nature of the Unfolded Ensemble: From Internal Friction to Conformational Landscapes"	Beijing, China
Jul 21, 2013	**7th International Discussion Meeting on Relaxations in Complex Systems (7th IDMRCS)**, "Insight into the molecular origins of the internal friction in unfolded proteins"	Barcelona, Spain
Jul 10, 2013	**Plenary Talk: Harvard Medical School Sixth International Epigenomics, Sequencing & SNiPs-2013 Meeting**, "Acetylations of Lysines of the H4 Histone Tail Lead to Major Remodeling of its Energy Landscape"	Boston, MA
June 6, 2013	**International Workshop and School Computational and theoretical modeling of macromolecular interaction**, "Multiscale Computational Modeling of Protein Folding and Dynamics"	Dubna, Russia
May 27, 2013	**Physics of Nucleic Acids**, "High-Resolution Coarse-Grained Modeling of DNA, Proteins and Their Complexes"	Yerevan, Armenia
May 17, 2013	**Institute for Mathematics and its Applications (IMA) at the University of Minnesota Stochastic Modeling of Biological Processes**, "Simulating cytoskeletal dynamics at high spatial and structural resolutions"	Minneapolis, MD

Feb 2, 2013	**Biophysical Society National Meeting, IDP Symposium**, "Acetylations of Lysines of the H4 Histone Tail Lead to Functionally Important Remodeling of its Energy Landscape"	Philadelphia, PA
Jan 18, 2013	**UMD-NCI Workshop of the Partnership for Cancer Technology**, "Physical Consequences of Posttranslational Modifications"	College Park, MD
Dec 15, 2012	**American Society For Cell Biology**, "Simulating cytoskeletal dynamics in lamellipodia and filopodia at high spatial and structural resolutions"	San Francisco, CA
Oct 15, 2012	**MMM2012 - Sixth International Conference on Multiscale Materials Modeling**, "Multi-Scale Modeling of DNA, Proteins and Their Complexes "	Singapore
Jul 19, 2012	**International Workshop on "The Emerging Dynamic View of Proteins: Protein Plasticity in Allostery, Evolution, and Self-Assembly" (DYPROT12)**, "Energy landscapes view of protein functional dynamics"	Dresden, Germany
Mar 25, 2012	**243rd American Chemical Society National Meeting**, "Secondary structure preferences of free histone tails and structural transitions induced upon binding to DNA"	San Diego, CA
Feb 28, 2012	**American Physical Society March Meeting 2012**, "Postranslational modifications significantly alter the binding-folding pathways of proteins associating with DNA"	Boston, MA
Jan 9, 2012	**Gordon Research Conference on Protein Folding Dynamics**, "Exploring Protein and DNA Energy Landscapes with Atomistic and Coarse-Grained Simulations"	Ventura, CA
Oct 30, 2011	**International Biophysics Congress (17th IBC)**, "Mesoscopic Physics of Eukaryotic Cell Motility"	Beijing, China
Oct 24, 2011	**Stochastic Processes in Cell and Population Biology, Mathematical Biosciences Institute (MBI)**, "Physico-Chemical Simulations of Eukaryotic Cell Motility"	Columbus, OH
Sep 11, 2011	**DNA Search: from Biophysics to Cell Biology**, "Atomistic and Coarse-Grained Simulations of DNA, Proteins and Protein-DNA Complexes"	Safed, Israel
Aug 12, 2011	**Rise of the Machines:Integration of experiment, simulation and theory for a mechanistic understanding of biomolecular machines** "A theory of motor-driven transport in cellular protrusions"	Telluride, CO
Jul 11, 2011	**The Physics, Chemistry, and Biology of Ions and Osmolytes in Solution** "Understanding the Behavior of Ions and Solvent near Nucleosome Particle, Histone Tails, and DNA"	Telluride, CO
June 2, 2011	**Biological Frontiers of Polymer and Soft Matter Physics**, "Mesoscopic Physics of Motile Protrusions in Eukaryotic Cells"	Santa Barbara, CA
Apr 7, 2011	**Design of Drugs and Chemicals that Influence Biology**, "Exploring Protein Energy Landscapes with Simulations: Applications to Histone Tails and Allosteric Transitions"	Los Angeles, CA

Dec 18, 2010	**The Pacifichem 2010 Congress**, "Accounting for hydration forces in coarse-grained biomolecular simulations"	Honolulu, HI
Aug 28, 2010	**Beckman Young Investigator Symposium**, "Multi-Scale Modeling of DNA and Chromatin"	Irvine, CA
Aug 9, 2010	**Plenary Talk: The Fourth Shanghai International Conference on Biophysics and Molecular Biology**, "Microscopic Physico-Chemical Modeling of Eukaryotic Cell Motility"	Shanghai, China
Jun 17, 2010	**Telluride Science Research Center: Characterizing Landscapes: From Biomolecules to Cellular Networks** , "Physico-Chemical Modeling of Actin Polymerization In Vivo"	Telluride, CO
Jun 8, 2010	**From Computational Biophysics to Systems Biology (CBSB)** , "Physico-Chemical Modeling of Actin Polymerization In Vivo"	Traverse City, MI
May 21, 2010	**An International Symposium on Solvation and Ionic Effects in Biomolecules: Theory to Experiment**, "Atomistic and Coarse-Grained Modeling of DNA and Chromatin"	Tsakhkadzor, Armenia
Oct 26, 2009	**Plenary Talk: American Chemical Society Southeastern Regional Meeting**, "Multi-Scale Approach to Understanding Physics of DNA and Nucleosome"	San Juan, Puerto Rico
Sep 12, 2009	**Workshop on Theory and Applications of Multi-Scale Modeling**, "A Molecular Renormalization Group Approach to Connecting Simulations at Different Scales"	Durham, NC
May 15, 2009	**Southeastern Theoretical Chemistry Association**, "Atomistic and Coarse-Grained Modeling of DNA and Chromatin."	Durham, NC
Apr 5, 2009	**American Mathematical Society Spring Meeting**, "Stochastic Dynamics of Cell Signaling and Cell Motility."	Raleigh, NC
Feb 2, 2009	**Mesilla Chemistry Workshop: Multi-Scale Modeling of Biological Molecules**, "Towards Physical Modeling of Complex Biophysical Processes from Chromatin Folding to Cell Motility."	Mesilla, NM
Apr 12, 2008	**American Chemical Society National Meeting**, "Mapping protein free energy landscapes from atomistic simulations"	New Orleans, LA
Mar 28, 2008	**Telluride Workshop on Mechanistic Analysis of Biological Systems**, "Building Biomolecular Coarse-Grained Force Fields from Atomistic Simulations"	Telluride, CO
Oct 26, 2007	**Chemistry at the Interface of Biology: Rising Stars in the Southeast - American Chemical Society Southeastern Regional Meeting**, "Towards Coarse-Grained Models of DNA and Chromatin from Atomistic Simulations"	Greenville, SC
Sep 20, 2007	**2nd annual Systems Biology Symposium, The Duke Center for Systems Biology**, "Stochastic Dynamics of Filopodial Growth"	Durham, NC
Mar 13, 2007	**Molecular Theory for Real Systems**, Ministry of Education and Science, Japan, "Towards Coarse-Grained Models of DNA and Proteins from Explicit Solvent Molecular Dynamics Simulations"	Nagoya, Japan

Nov 14, 2006	**The Global Dialogues on Emerging Science and Technology (GDEST) Conference on Bioinformatics**, "Physical Bioinformatics: from the Hydrophilic Code in Proteins to Chromatin Regulation Mechanisms"	Petropolis, Brazil
Aug 1, 2006	**SIAM Conference on the Life Sciences**, "New Approaches to Studying Stochastic Chemical Kinetics in Biochemical Reaction Networks"	Raleigh, NC
Nov 3, 2004	**Triangle Biophysics Symposium**, "Bioinformatics Meets Physics: Improving Protein Modeling Algorithms"	Research Triangle Park, NC
May 15, 2003	**International Workshop on "Proteomics: Protein Structure, Function, and Interactions",** "Recognition in biomolecular energy landscapes: protein association vs protein folding"	Trieste, Italy
Apr 10, 2002	**American Chemical Society National Meeting**, "Binding and Folding: an Energy Landscape Perspective"	Orlando, FL

Universities & Research Centers

Mar 10, 2016	**George Washington University** "Molecular Simulations of Mechanochemical Dynamics of the Cellular Cytoskeleton"	Washington, DC
Apr 27, 2015	**University of Oregon**, "The Chromatin Folding Problem: Computer Simulations of Nucleosomes and Histone Tails"	Eugene, Oregon
Apr 22, 2015	**New York University**, "Computational Modeling of the Acto-Myosin Cytoskeleton"	New York, NY
Apr 17, 2015	**Pennsylvania State University** , "The Chromatin Folding Problem: Computer Simulations of Nucleosomes and Histone Tails"	University Park, PA
Apr 8, 2015	**Higher Chemical College, Russian Academy of Sciences** , "Computational Modeling of Protein Binding: Theory and Applications"	Moscow, Russia
Dec 15, 2014	**Basque Center for Applied Mathematics**, "Computational Modeling of the Eukaryotic Cytoskeleton"	Bilbao, Spain
Oct 15, 2014	**Oxford University**, "Computational Modeling of the Eukaryotic Cytoskeleton"	Oxford, UK
Jun 12, 2014	**Moscow Institute of Physics and Technology**, "Binding and Folding Landscapes of Ubiquitin, Histones and Their Chaperones"	Moscow, Russia
Apr 9, 2014	**Rice University**, "Computational Modeling of the Eukaryotic Cytoskeleton"	Houston, Texas
Apr 8, 2014	**University of Houston**, "The Chromatin Folding Problem: Computer Simulations of Nucleosomes and Histone Tails"	Houston, Texas
Dec 19, 2013	**National Institute of Health, NIDDK** "Using Computer Simulations to Study the Dynamics of Unfolded Proteins and the Ubiquitin Dimer"	Bethesda, MD

Dec 6, 2013	**National Institute of Health, NCBI**, "The Chromatin Folding Problem: Computer Simulations of Nucleosomes and Histone Tails"	Bethesda, MD
Nov 13, 2013	**Massachusetts Institute of Technology**, "Computer Simulations of Cytoskeletal Dynamics and Cell Motility"	Boston, MA
Sep 19, 2013	**Boston College**, "Atomistic and Coarse-Grained Simulations of Histones, DNA and Nucleosomes "	Boston, MA
Aug 5, 2013	**Beijing University**, "Towards Understanding of the Way DNA is Compacted in Nuclei of Cells"	Beijing, China
Feb 13, 2013	**Johns Hopkins University School of Medicine** , "Energy landscapes' approaches to understanding protein dynamics"	Baltimore, MD
Nov 30, 2012	**Virginia Tech**, "Computational Modeling of Actin Network Self-Assembly and Dynamics"	Blacksburg, VA
Sep 26, 2012	**Yerevan State University** , "The Chromatin Folding Problem: How DNA is Compacted in Nuclei of Cells"	Yerevan, Armenia
Jul 11, 2012	**Max Planck Institute for the Physics of Complex Systems** , "Theory of Active Transport in Filopodia and Stereocilia"	Dresden, Germany
Jun 18, 2012	**Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic** , "Towards Computer Simulations of Chromatin Folding"	Prague, Czech Republic
Jun 14, 2012	**Oxford University, Department of Physics** , "Towards Computer Simulations of Chromatin Folding"	Oxford, England
Jun 6, 2012	**Oxford University, The Oxford Centre for Collaborative Applied Mathematics (OCCAM)** , "Mechano-chemical feedbacks govern stochastic dynamics of actin networks in eukaryotic cells"	Oxford, England
Feb 23, 2012	**Mount Sinai School of Medicine** "The Chromatin Folding Problem: Studying Nucleosomes, Histone Tails and DNA Using Atomistic and Coarse-Grained Simulations"	New York, NY
Jan 17, 2012	**Korea Advanced Institute of Science and Technology (KAIST)**, "The Chromatin Folding Problem: Atomistic and Coarse-Grained Simulations of DNA, Histone Tails and Nucleosomes"	Muju, South Korea
Nov 2, 2011	**Tsinghua University**, "'Detailed Physico-Chemical Modeling of Cytoskeletal Dynamics and Motility in Eukaryotic Cells"	Beijing, China
Oct 3, 2011	**The University of Texas at Austin**, "Atomistic and Coarse-Grained Simulations of Nucleosomes, Proteins and DNA"	Austin, TX
Sep 26, 2011	**George Mason University**, "Atomistic and Coarse-Grained Simulations of DNA, Proteins and Protein-DNA Complexes"	Fairfax, VA
May 19, 2011	**National Institute of Health**, "Mapping biomolecular free energy landscapes from atomistic and coarse-grained simulations"	Bethesda, MD
Jan 21, 2011	**Center for Bioinformatics and Computational Biology, University of Maryland**, "Atomistic and Coarse-Grained Simulations of DNA and Nucleosomes"	College Park, MD
Jan 19, 2011	**Informal Statistical Physics Seminar, University of Maryland**, "Principles of active transport in filopodia"	College Park, MD

Nov 15, 2010	**Duke University**, "Stochastic Modeling of Actin Polymerization in Vivo"	Durham, NC
Oct 15, 2010	**The University of Texas at Arlington**, "Mechano-chemical feedbacks finely regulate actin polymerization processes in vivo"	Arlington, TX
May 24, 2010	**Yerevan State University**, "Physical Modeling of Eukaryotic Cell Motility"	Yerevan, Armenia
Jan 19, 2010	**University of Maryland**, "Towards Physical Modeling of Complex Biophysical Processes from Chromatin Folding to Cell Motility"	College Park, MD
Dec 11, 2009	**Rensselaer Polytechnic Institute**, "Exploring Functional Landscapes of Proteins"	Troy, NY
Sep 10, 2009	**North Carolina A&T State University**, "Understanding electrostatic and hydration interactions governing nucleosomal core particle and flexible histone tails"	Greensboro, NC
Apr 2, 2009	**Cornell University**, "Towards Physical Modeling of Complex Biophysical Processes from Chromatin Folding to Cell Motility"	Ithaca, NY
Mar 13, 2009	**University of California at San Diego**, "Towards Physico-Chemical Description of Eukaryotic Cell Motility."	San Diego, CA
Nov 27, 2008	**University of Toronto**, "Energy Landscapes View of Protein Native Dynamics."	Toronto, Canada
Nov 7, 2008	**University of Richmond**, "Multi-Scale Modeling of DNA and Chromatin."	Richmond, VA
Sep 11, 2008	**University of Pennsylvania**, "Towards Physical Modeling of Complex Biophysical Processes from Chromatin Folding to Cell Motility."	Philadelphia, PA
Nov 26, 2007	**North Carolina State University, Department of Physics**, "Towards Coarse-Grained Models of DNA and Chromatin from Atomistic Simulations"	Raleigh, NC
Nov 19, 2007	**Bioinformatics and Computational Biology Program Seminars**, "Understanding the hierarchical organization of protein dynamics from atomistic simulations"	UNC-Chapel Hill
Apr 26, 2007	**Duke University**, "Towards Computational Modeling of Chromatin: Insights into DNA Electrostatics from Molecular Dynamics Simulations"	Durham, NC
Mar 14, 2007	**Nagoya University**, "Stochastic Signaling in Nonlinear Enzyme Cascades"	Nagoya, Japan
Mar 12, 2007	**Kyoto University**, "Insights into DNA Electrostatics and Counterionic Atmosphere Details from Computer Simulations"	Kyoto, Japan
Feb. 6, 2007	**The University of Wisconsin-Madison**, "Exploring Protein Energy Landscapes with Free Energy Techniques."	Madison, WS
Nov 29, 2006	**Rice University**, "Towards Computational Modeling of Chromatin: Molecular Dynamics Simulations of Counterion Condensation around DNA"	Houston, TX

Mar 29, 2006	**North Carolina State University, Department of Chemical Engineering**, "Similarities and differences in Na+ and K+ condensation around DNA"	Raleigh, NC
Sep 22, 2005	**Biophysics Program Seminars**, "Physical Chemistry of Cellular Processes: From DNA Electrostatics to Signal Transduction"	UNC-Chapel Hill
Oct 18, 2004	**Moscow State University, Department of Physics**, "Water in Biomolecular Recognition Landscapes"	Moscow, Russia

CONTRIBUTED LECTURES

Jul 21, 2015	**The 10th European Biophysics Congress**, "The Acetylation Landscape of the H4 Histone Tail"	Dresden, Germany
Mar 3, 2014	**2014 American Physical Society March Meeting** , "What is the Origin of Internal Friction in Unfolded Proteins?"	Denver, CO
Mar 21, 2010	**American Chemical Society National Meeting**, "Multiscale approach to modeling of DNA and chromatin"	San Francisco, CA
Nov 25, 2009	**Expanding the frontiers of molecular dynamics simulations in biology Joint BSC - IRB Barcelona Conference**, "Intrinsic Conformational Preferences of Disordered Histone Tails"	Barcelona, Spain
Aug 18, 2009	**American Chemical Society National Meeting**, "Energy landscapes analysis of disordered proteins: A case study of histone tail dynamics"	Washington, DC
Mar 12, 2008	**American Physical Society National Meeting**, "Stochastic Dynamics of Filopodial Growth"	New Orleans, LA
Mar 5, 2007	**American Physical Society National Meeting**, "Stochastic Chemical Kinetics in Biochemical Reaction Networks"	Denver, CO
Sep 13, 2006	**American Chemical Society National Meeting**, "Free Energies of Protein Conformations from All-Atom Molecular Dynamics Simulations"	San Francisco, CA