# GAREGIN A. PAPOIAN

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## APPOINTMENTS

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| 2014-Present | Monroe Martin Professor, Department of Chemistry and Biochemistry & Institute for Physical Science and Technology , University of Maryland | College Park, MD |
| 2014-2019 | 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<br>NIH Postdoctoral Research Associate; *Adviser: Prof. P. G. Wolynes* | La Jolla, CA |
| 2000 | Department of Chemistry, The University of Pennsylvania<br>Postdoctoral Research Associate; *Adviser: Prof. M. L. Klein* | Philadelphia, PA |
| 1995-1999 | Department of Chemistry, Cornell University<br>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 |
| 1988-1990 | High School of Physics & Mathematics | Yerevan, Armenia |

## HONORS AWARDS

| | | |
|---|---|---|
| 2019 | • Visiting Merton Fellow (University of Oxford) | Oxford, UK |
| 2016 | • Visiting Fellow of the Isaac Newton Institute for Mathematical Sciences, Cambridge University, UK | Cambridge, UK |
| 2011 | • Rice Family Fellowship, The Kavli Institute for Theoretical Physics | Santa Barbara, CA |
| 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 |

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|---|---|---|
| 1995 | • H. P. Cady Award for Academic Excellence, The University of Kansas | Lawrence, KS |
| 1992 | • Mendeleev Award for Outstanding Undergraduate Student Research in Russia | 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

Google Scholar, h-index: **34**; Total Citations: **4,031**

⋆ denotes manuscripts where G. A. Papoian was among the corresponding authors

### UMD

**2020**

⋆91. C. Floyd, H. Levine, C. Jarzynski and G. A. Papoian,, "Driven-dissipative dynamics of active cytoskeletal networks underlie near-critical energy fluctuations", **Nature Physics**, (2020), submitted, arXiv:2006.01884

90. S. Jin, V. G. Contessoto, M. Chen, N. P. Schafer, W. Lu, X. Chen, C. Bueno, A. Hajitaheri, B. J. Sirovetz, A. Davtyan, G. A. Papoian, M.Y. Tsai, and P. G. Wolynes, "AWSEM-Suite: a protein structure prediction server based on template-guided, coevolutionary-enhanced optimized folding landscapes", **Nucleic Acids Res**, (2020), 10.1093/nar/gkaa356

89. X. Li, Q. Ni, X. He, J. Kong, S.M. Lim, G. A. Papoian, J. P. Trzeciakowskic, A. Trachec, and Y. Jiang, "Tensile Force Induced Cytoskeletal Reorganization: Mechanics Before Chemistry", **PLOS Comp Bio**, (2020), 16 (6), e1007693, DOI: 10.1371/journal.pcbi.1007693

⋆88. C. Floyd,Y Dalal, G. A. Papoian, and C. Jarzynski, "Gibbs Free Energy Change of a Discrete Chemical Reaction Event", **J Chem Phys**, (2020), 152 (8), 084116, DOI: 10.1063/1.5140980 **(Editor's Pick)**

⋆87. M. Pitman,Y Dalal, and G. A. Papoian, "Minimal Cylinder Analysis Reveals the Mechanical Properties of Oncogenic Nucleosomes", **Biophys J**, (2020), 118, 2309-2318, DOI: 10.1016/j.bpj.2020.01.042

**2019**

⋆86. D. P. Melters, M. Pitman, T. Rakshit, S. A. Grigoryev, M. Bui1, D. Sturgill, G. A. Papoian, and Y Dalal,, "Intrinsic Elasticity of Nucleosomes is Encoded by Histone Variants and Calibrated by their Binding Partners", **Proc Nat Acad Sci USA**, (2019), 116, 24066-24074 DOI: 10.1073/pnas.1911880116

⋆85. Q. Ni, G. A. Papoian, "Turnover versus Treadmilling in Actin Network Assembly and Remodeling", **Cytoskeleton**, (2019), 76 (11-12), 562-570 DOI: 10.1002/cm.21564

⋆84. A. Chandrasekaran, A. Upadhyaya, G. A. Papoian, "Remarkable Structural Transformations of Actin Bundles are Driven by their Initial Polarity, Motor Activity, Crosslinking, and Filament Treadmilling", **PLOS Comp Bio**, (2019), 15, e1007156, DOI: 10.1371/journal.pcbi.1007156

⋆83. H. Zhang, D. Winogradoff, Y. Dalal, G. A. Papoian, "The Oligomerization Landscape of Histones", **Biophys J**, (2019), 116, 1845-1855

⋆82. C. Floyd, G. A. Papoian and C Jarzynski "Quantifying Dissipation in Actomyosin Networks", **Interface Focus**, (2019), v 9, 10.1098/rsfs.2018.0078, (**Journal Cover**, Interface Focus, Volume 9, Issue 3, April 19, 2019)

**2018**

⋆81. J. Komianos and G. A. Papoian "Stochastic Ratcheting on a Funneled Energy Landscape is Necessary for Highly Efficient Contractility of Actomyosin Force Dipoles", **Phys Rev X**, (2018), 8, 021006, DOI: 10.1103/PhysRevX.8.021006

⋆80. H. Wu, P. G. Wolynes and G. A. Papoian "AWSEM-IDP: A Coarse-Grained Force Field for Intrinsically Disordered Proteins", **J Phys Chem B**, (2018), 122, 11115-11125, DOI:10.1021/acs.jpcb.8b05791

**2017**

⋆79. C Floyd, C. Jarzynski and G. A. Papoian "Low-Dimensional Manifold of Actin Polymerization Dynamics", (2017), arXiv:1708.04695 [q-bio.SC]; **New J Phys**, (2017), 19, 125012 DOI 10.1088/1367-2630/aa964

⋆78. M. Bui , M. Pitman , A. Nuccio , S. Roque , P. Donlin-Asp , A. Nita-Lazar , G. A. Papoian and Y. Dalal, "Internal Modifications in the CENP-A Nucleosome Modulate Centromeric Dynamics", **Epigenetics Chromatin**, (2017), 10, 17, DOI 10.1186/s13072-017-0124-6

77. S. M. Avdoshenko, A. Das, R. Satija, G. A. Papoian, and D. E. Makarov, "Theoretical and Computational Validation of the Kuhn Barrier Friction Mechanism in Unfolded Proteins", **Sci Rep**, (2017), 7, 269, DOI:10.1038/s41598-017-00287-5

⋆76. D. Potoyan and G. A. Papoian, "The Need for Computational Speed: State of the Art in DNA Coarse Graining;" **Contributed Book Chapter in "Coarse-Grained Modeling of Biomolecules, Publisher CRC Press , edited by G. A. Papoian;** (2017), ISBN-10: 1466576065

⋆75. G. A. Papoian and P. G. Wolynes "AWSEM-MD: From Neural Networks to Protein Structure Prediction and Functional Dynamics of Complex Biomolecular Assemblies;" **Contributed Book Chapter in "Coarse-Grained Modeling of Biomolecules, Publisher CRC Press, edited by G. A. Papoian;** (2017), ISBN-10: 1466576065

⋆74. G. A. Papoian, "A Brief Historical Survey of Coarse-Graining of Biomolecules;" **Contributed Book Chapter in "Coarse-Grained Modeling of Biomolecules, Publisher CRC Press, edited by G. A. Papoian;** (2017), ISBN-10: 1466576065

73. I. Echeverria and G A. Papoian, "Perspectives on the Coarse-Grained Models of DNA", **Contributed Book Chapter in "Many-Body Effects and Electrostatics in Biomolecules, Publisher Pan Stanford; edited by Qiang Cui and Markus Meuwly;** (2017), ISBN-10: 9814613924

**2016**

⋆72. H. Zhao, D. Winogradoff, M. Bui, Y. Dalal, G. A. Papoian, "Promiscuous Histone Mis-Assembly is Actively Prevented by Chaperones", **J Am Chem Soc**, (2016), 138, 13207-13218 (Journal Cover, JACS, Volume 138, Issue 40, October 12, 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), 138, 8126-8133

⋆70. K. Popov, J. Komianos, G. A. Papoian "MEDYAN: Mechanochemical Simulations of Contraction and Polarity Alignment in Actomyosin Networks", **PLOS Comp Bio**, (2016), DOI:10.1371/journal.pcbi.1004877

⋆69. U. Dobramysl, G. A. Papoian, and R. Erban "Steric Effects Induce Geometric Remodeling of Actin Bundles in Filopodia", **Biophys J**, (2016), 110, 2066-2075

⋆68. A. Davtyan, M. Platkov, M. Gruebele, G. A. Papoian, 'Stochastic Resonance in Protein Folding Dynamics", **ChemPhysChem**, (2016), DOI: 10.1002/cphc.201501125

⋆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. Fondrie, 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-$\kappa$B-Nuclear Localization Signals by I$\kappa$B$\alpha$ and I$\kappa$B$\beta$", **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

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 $\alpha/\beta$ 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. Norskov, 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]para-cyclophane 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** | |
| 2018-Present | **F1000Prime**, The inaugural Section Head for Theory & Modeling in Biological Physics |
| 2016-Present | **Scientific Reports (Nature Group)**, Editorial Board Member |
| **Scientific Societies** | |
| 2016-2017 | **Intrinsically Disordered Proteins (IDP) Subgroup of the Biophysical Society**, Chair |
| **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; 2014-2019); 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, 2015-2018); Executive Committee (Chemistry and Biochemistry; 2012-2016); Q-Bio Cluster Hire Search Committee (2012-2014) |

## CONFERENCE ORGANIZER

| | | |
|---|---|---|
| Oct 16, 2019 | Global Innovation Forum 2019 | Yerevan, Armenia |
| July 17, 2018 | Telluride Science Research Center: Protein and Peptide Interactions in Cellular Environments; *Meeting Co-Chairs: Scott Showalter and Garegin Papoian* | Telluride, CO |
| May 9, 2017 | Mechanobiology of the Cytoskeleton: Molecular and Cellular Principles; *Meeting Co-Chairs: Arpita Upadhaya and Garegin Papoian* | College Park, MD |
| 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 |

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|---|---|---|
| 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-1800418**
(PI: Papoian)
"Molecular Simulations of Biological Active Matter"
04/01/2018-03/31/2021

**National Science Foundation, PHY-1806903**
(PI; Upadhyaya; co-PIs: Papoian, Losert)
"Collaborative Research: Formation of a High Flux Student Research Network (HF-SRN) as a Laboratory for Enhancing Interaction in the PoLS SRN"
09/12/2018-09/11/2023

**Amazon AWS Artificial Intelligence Award**
(PI; Papoian)
"Predicting Protein Structures by Integrating Deep Learning and Energy Landscapes Perspectives"
01/1/2018-1/1/2020

## COMPLETED FUNDING

**National Science Foundation, PHY-1206060**
(PI; Upadhyaya; co-PI: Papoian)
"Physics of Centrosome Reorientation During Signaling Activation in Immune Cells"
09/15/2016-08/31/2019

**National Science Foundation, CHE-1363081**
(PI: Papoian)
"Mechanochemistry of Actin Networks"
06/01/2014-08/31/2017

**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

**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

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|---|---|---|
| Fall 2020 | "Fundamentals of General Chemistry" | Chem 131 |
| Spring 2018 | "Physical Chemistry I" | Chem 481 |
| Fall 2017 | "Fundamentals of General Chemistry" | Chem 131 |
| Fall 2016 | "Chemical and Statistical Thermodynamics" | Chem 684 |
| 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 |

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| 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**

| | |
|---|---|
| 2014-Present | *Hao Wu*, Biophysics Program |
| 2014-Present | *Mary Pitman*, Chemistry Program |
| 2015-Present | *Aravind Chandrasekaran*, Chemistry Program |
| 2016-Present | *Qin Ni*, Chemical Engineering |
| 2016-Present | *Cal Floyd*, Biophysics |
| 2017-Present | *Haoran Ni*, Biophysics |

## FORMER GROUP MEMBERS

**Graduate Students**

| | | |
|---|---|---|
| 2012-2018 | *Haiqing Zhao*, Thesis Title: "Uncovering the Biophysical Mechanisms of Histone Complex Assembly"; currently a postdoctoral fellow at Columbia University | Ph.D., 2018 |
| 2013-2018 | *James Komianos*, B.S. Carnegie Mellon University, Thesis Title: "Uncovering Fundamental Mechanisms of Actomyosin Contractility Using Analytical Theory and Computer Simulations"; Currently a financial engineer at a private company | Ph.D., 2018 |
| 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. A. Kolomeiski at the Rice University | Ph.D., 2013 |

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|---|---|---|
| 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 the Caldwell Assistant Professor, Department of Chemistry, Iowa State 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 data scientist at a private company | 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 |

**Postdoctoral Associates**

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| 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 a Professor in the Department of Physics at Beijing University of Posts and Telecommunications, China |
| 2005-2007 | *Dr. Sangwook Wu* is currently an Assistant Professor in the Department of Physics at Pukyong National University in Busan, South Korea |
| 2005-2010 | *Dr. Alexey Savelyev* is currently a researcher at the University of Texas, Health Science Center, San Antonio |

**Undergraduate Students**

| | | |
|---|---|---|
| 2018-2019 | *Kareem McDavid*, UMD College Park | Junior |
| 2016-2018 | *Robert Liu*, UMD College Park | Sophomore |
| 2015-2016 | *Jeffrey Wang*, UMD College Park | Junior |
| 2011-2014 | *Michelle Thomas (Beckman Scholar)*, UMD College Park | Sophomore |

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|---|---|---|
| 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 |

## INVITED LECTURES

### Conferences

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| Jan 23, 2020 | **"Winter School on Physics of the Cell"**, "Mechanochemical Modeling of Acive Matter" | Trento, Italy |
| Jan 23, 2020 | **"Winter School on Physics of the Cell"**, "Mechanochemical Modeling of Acive Matter" | Trento, Italy |
| Nov 5, 2019 | **"EUTOPIA 2019"**, "Emergence of Contractility in Acto-Myosin Networks" | San Sebastian, Spain |
| Oct 24, 2019 | **"CECAM Workshop: Protein simulations – current state of the art"**, "Modulating Nucleosomal Elasticity as a Novel Axis of Epigenetic Regulation" | Tel Aviv, Israel |
| Oct 18, 2019 | **"FAST: Global Innovation Forum 2019"**, "Towards Simulating Cells of Higher Organisms from the First Principles" | Yerevan, Armenia |
| Oct 12, 2019 | **"Science and Technology Convergence Conference"**, "Towards Predictive Computational Modeling of Human Cells from the First Principles" | Yerevan, Armenia |
| Jul 21, 2019 | **Multiscale modeling of cytoskeleton-mediated cellular transport and aggregation, 2019 SMB Annual Meeting**, "Entropy Production and Cytoskeletal Avalanches in Actin Networks" | Montreal, Canada |
| Jul 8, 2019 | **NSF iPOLS Meeting**, "Towards Simulating Eukaryotic Cells from the Fundamental Physico-Chemical Principles" | Munich, Germany |
| Mar 31, 2019 | **The Biophysical Society Thematic Meeting: Multiscale Modeling of Chromatin: Bridging Experiment with Theory**, "Structural Plasticity of Histone Oligomers and Their Interactions with Chaperones and Other Regulators" | Les Houches, France |
| Feb 1, 2019 | **Multiscale Simulations and Mathematical Modelling of Complex Biological Systems**, "Towards Simulating Eukaryotic Cells from the Fundamental Molecular Principles" | New Delhi, India |
| Oct 27, 2018 | **Computational Biophysics at the Molecular and Mesoscales, 14th Rencontres du Vietnam**, "Towards Simulating Eukaryotic Cells from the Fundamental Molecular Principles" | Quy Nhon, Vietnam |

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| Oct 25, 2018 | **The First ICST Workshop on Computational Biophysics and Medicine**, "Modeling Biomolecular Structure and Dynamics by Blending Ideas from Machine Learning and Physics" | Ho Chi Minh City, Vietnam |
| Oct 15, 2018 | **The Society of Rheology 90th Annual Meeting**, "Fundamental Principles behind the Emergence of Contractility in Acto-Myosin Networks " | Houston, TX |
| Sep 29, 2018 | **Brazilian Biophysical Society Annual Meeting**, "Assembly and Dynamics of Histone Oligomers and Nucleosomes" | Brazil |
| Sep 24, 2018 | **Royal Society Theo Murphy Meetings 2018, "Multi-Resolution Simulations of Intracellular Processes"**, "Towards Simulating Eukaryotic Cells at Single Molecule Resolution" | Chicheley, UK |
| Aug 12, 2018 | **BIRS Workshop: Mathematics of the Cell: Mechanical and Chemical Signaling across Scales**, "Theory of Active and Passive Force Dipoles in Contractile Acto-Myosin Networks" | Banff, Canada |
| Aug 6, 2018 | **SIAM Conference on the Life Sciences: Modeling Cell Motility and Cytoskeleton Interactions**, "Understanding the Emergence of Contractility in Acto-Myosin Networks" | Minneapolis, MN |
| Jul 19, 2018 | **Protein-Peptide TSRC workshop**, "Coarse-Grained and Atomistic Modeling of Histone Tails and Cores, Nucleosomes and Their Modifications" | Telluride, CO |
| Jul 10, 2018 | **Biophysical Dynamics workshop**, "Theory of Active and Passive Force Dipoles in Contractile Acto-Myosin Networks" | Telluride, CO |
| Jul 9, 2018 | **Water: Grand Challenges for Molecular Science and Engineering**, "Water-Mediated Interactions in Protein and Protein-DNA Complexes" | Telluride, CO |
| June 26, 2018 | **The Nordic Institute for Theoretical Physics: Generation and Control of Forces in Cells**, "Theory of Active and Passive Force Dipoles in Contractile Acto-Myosin Networks" | Stockholm, Sweden |
| Mar 12, 2018 | **Polyelectrolytes in Chemistry, Biology and Technology 2018**, "Multiscale Studies of Nucleosomal Assembly and Dynamics" | Singapore |
| Jan 7, 2018 | **Gordon Research Conference on Protein Folding Dynamics**, "Physics and Biology of Nucleosomal Assembly and Dynamics" | Galveston, TX |
| Oct 18, 2017 | **Workshop on Machine Learning for Discovery Science**, "Protein Structure Prediction: Blending Ideas from Machine Learning and Physics" | Yerevan, Armenia |
| Oct 7, 2017 | **Coarse graining of biomolecules and beyond: theory and applications,**, "AWSEM-MD: Overview of the Force Field and Selected Applications " | Warsaw, Poland |
| Aug 22, 2017 | **American Chemical Society National Meeting**, "Understanding the Emergence of Contractility in Acto-Myosin Networks" | Washington, DC |
| Jun 25, 2017 | **2017 Annual Meeting of the International Physics of Living Systems (iPoLS) Network**, "Elucidating Physical Principles Giving Rise to the Emergence of Contractility in Disordered Acto-Myosin-Crosslinker Networks" | Paris, France |

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| Jun 20, 2017 | **Physics and Biology of Proteins**, "Coarse-Grained Modeling of Biomolecules: A Brief History and Overview" | Natal, Brazil |
| Jun 19, 2017 | **Physics and Biology of Proteins**, "Structure and Dynamics of Nucleosomes from Atomistic and Coarse-Grained Simulations" (**Keynote Presentation**) | Natal, Brazil |
| May 9, 2017 | **Biophysics Symposium: Mechanobiology Of The Cytoskeleton - Molecular And Cellular Principles** , "Understanding the Emergence of Contractility in Actomyosin Networks" | College Park, MD |
| Apr 2, 2017 | **Modeling and experimental approaches to genome organization: from DNA to chromatin and chromosomes, epigenetics and cellular function**, "Atomistic and Coarse-Grained Simulations of Centromeric and Canonical Histone Complexes, Nucleosomes and Their Chaperones" | Les Houches, France |
| Nov 28, 2016 | **3rd International Conference on Computational Science and Engineering**, "Towards Understanding Complex Protein Dynamics in vivo" | Ho Chi Minh city, Vietnam |
| Nov 21, 2016 | **ISCB-LA2016**, "Biomolecular Dynamics in Complex in vivo Environments" | Buenos Aires, Argentina |
| Oct 14, 2016 | **Regional Meeting of the Biophysical Society**, "Towards Understanding the Mechano-Chemical Dynamics of the Eukaryotic Cytoskeleton" (**Keynote Presentation**) | Lehigh University |
| Oct 2, 2016 | **"Mechanical Behaviors of Cytoskeleton and Cells" Symposium of The Society of Engineering Science 53rd Annual Technical Meeting,** , "Mechanochemical Modeling of the Eukaryotic Cytoskeleton" | College Park, MD |
| Aug 21, 2016 | **"Intrinsically Disordered Proteins: Structure, Function, and Interactions," 252nd American Chemical Society National Meeting**, "Atomistic and Coarse-Grained Modeling of Histone Cores and Tails" | Philadelphia, PA |
| Jun 27, 2016 | **Protein and Peptide Interactions in Cellular Environments**, "Complexity of Biomolecular Processes in Cells" | Telluride, CO |
| May 23, 2016 | **Hong Kong University of Science and Technology IAS Focused Program on Molecular Machines of Life: Simulation Meets Experiment**, "Computational Modeling of Histone Complexes, Nucleosomes and Their Modifications" | Hong Kong, China |
| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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**

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| Dec 11, 2019 | **Department of Physics, Leeds University**, ""Mechanochemical Modeling of Acive Matter" | Leeds, UK |
| Nov 1, 2019 | **Mathematical Biology and Ecology Seminar, Oxford University**, "Nucleosomal Elasticity as a Novel Axis of Epigenetic Regulation " | Oxford, UK |
| Oct 31, 2019 | **Industrial and Applied Mathematics Seminar, Oxford University** , "Towards Simulating Eukaryotic Cells from the Fundamental Physico-Chemical Principles" | Oxford, UK |
| Oct 13, 2019 | **Institute of Molecular Biology**, "Mechanical Properties of Nucleosomes from *in silico*, *in vitro* and *in vivo* Studies" | Yerevan, Armenia |
| Apr 16, 2019 | **The Courant Institute, New York University**, "Towards Simulating Eukaryotic Cells from the Fundamental Molecular Principles" | New York City, NY |
| Oct 19, 2018 | **Georgia State University**, "Towards Simulating Eukaryotic Cells from the Fundamental Molecular Principles" | Atlanta, GA |
| Jun 25, 2018 | **University of Zurich**, "Modeling Biomolecular Structure and Dynamics by Blending Ideas from Machine Learning and Physics" | Zurich, Switzerland |
| Apr 19, 2018 | **Stony Brook University** "Simulating Biophysical Processes from Nanometers to Microns: From Proteins and Nucleosomes to Cellular Scale Cytoskeletal Dynamics" | Stony Brook, NY |
| Nov 11, 2017 | **University of Pennsylvania** , "Learning the Molecular Principles Underlying Dynamics of the Eukaryotic Cytoskeleton" | Philadelphia, PA |

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| May 29, 2017 | **Lund University Dynamic structures: from atomic to cellular length scales**, "Simulating Biophysical Processes from Nanometers to Microns: From Proteins and Nucleosomes to Cellular Scale Cytoskeletal Dynamics" | Lund, Sweden |
| Oct 10, 2016 | **MIT**, "Complex Protein Dynamics in vivo" | Boston, MA |
| Sep 9, 2016 | **UMBC**, "Mechanochemical Modeling of Cytoskeletal Network Dynamics" | Baltimore, MD |
| May 17, 2016 | **Cambridge University, Gurdon Institute**, "Mechanochemical Organization of the Eukaryotic Cytoskeleton" | Cambridge, United Kingdom |
| 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 |

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| 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 |

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| 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 |