September 2019

Curriculum Vitae and Table of Contents

James C. Gumbart, Ph.D.
Associate Professor
School of Physics
Georgia Institute of Technology

March 2019

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Associate Professor
School of Physics
Georgia Institute of Technology

I. Earned Degrees

B.S. Physics & Mathematics	2000-2003	Western Illinois University, Macomb, IL
M.S. Physics	2003-2005	University of Illinois, Urbana-Champaign
Ph.D. Physics	2005-2009	University of Illinois, Urbana-Champaign (advisor: K. Schulten)

II. Employment History

2009-2010	Postdoctoral Associate, Beckman Institute UIUC (advisor: K. Schulten)
2011-2012	Director's Postdoctoral Fellow, Argonne National Laboratory (advisor: B. Roux)
2013-2018	Assistant Professor, School of Physics, Georgia Institute of Technology
2018-present	Associate Professor, School of Physics, Georgia Institute of Technology
2013-present	Adjunct faculty, School of Chemistry & Biochemistry and School of Biology, Georgia Institute of Technology

III. Honors and Awards

2019-2020	Hesburgh Award Teaching Fellow, Georgia Institute of Technology
2017-2018	Cullen-Peck Fellow, Georgia Institute of Technology
2017	DOE INCITE Award
2015-2020	NSF CAREER Award
2014	Research featured on the cover of Pittsburgh Supercomputing Center Spring '14 brochure
2011-2012	Director's Postdoctoral Fellowship, Argonne National Laboratory

IV. Research, Scholarship, and Creative Activities

(* next to item number indicates work done at Georgia Tech)
(**bold** indicates Gumbart group member; @ indicates undergraduate author; * indicates corresponding authorship)
Google Scholar profile at http://scholar.google.com/citations?user=DOMzcTgAAAAJ&hl=en

A. Published Books, Book Chapters, and Edited Volumes

A1. Books

No data

A2. Refereed Book Chapters

5. **Balusek C**, **Hwang H**, **Hazel A**, **Lundquist K**, **Pavlova A**, **Gumbart JC**. Diverse Protein-Folding Pathways and Functions of *β*-Hairpins and *β*-Sheets. In *Quantitative Models for Microscopic to Macroscopic Biological Macromolecules and Tissues*, L. Olivares-Quiroz and O. Resendis-Antonio, Eds. Springer, 1-20, 2018.
4. Nguyen LT, **Gumbart JC**, Jensen GJ. Coarse-grained simulations of bacterial cell wall. In *Bacterial Cell Wall Homeostasis: Methods and Protocols,* H.-J. Hong, Ed. Springer, 1440:247-270, 2016.
3. **Gumbart J**. Exploring substrate diffusion using biased molecular dynamics simulations. In *Methods in Molecular Biology*, N. Vaidehi and J. Klein-Seetharaman, Eds. Springer, 914:337-350, 2012.

2. **Gumbart J,** Schreiner E, Trabuco LG, Chan KY, Schulten K. Viewing the mechanisms of translation through the computational microscope. In *Molecular Machine in Biology*, J. Frank, Ed. Cambridge University Press, pp 142-157, 2011.
1. Wen PC, Huang Z, Enkavi G, Wang Y, **Gumbart J**, Tajkhorshid E. Molecular mechanisms of active transport across the cellular membrane. In *Molecular Simulations and Biomembranes: From Biophysics to Function,* P. Biggin and M. Sansom, Eds. RSC Press, pp 248-286, 2010.

A3. Edited Volumes

No data

B. Refereed Publications and Submitted Articles

B1. Published and Accepted Journal Articles

78*. Conformational dynamics of AcrA govern multidrug efflux pump assembly. **A. J. Hazel**, N. Abdali, I. V. Leus, J. M. Parks, J. C. Smith, H. I. Zgurskaya, and **J. C. Gumbart**. *ACS Infectious Diseases*. In press.

77*. Presence of substrate aids lateral gate separation in LptD. **K. P. Lundquist** and **J. C. Gumbart**. *Biochimica et Biophysica Acta (BBA) – Biomembranes*. In press.

76*. Tyrosine, cysteine, and proton coupled electron transfer in a ribonucleotide reductase-inspired beta hairpin maquette. T. G. McCaslin, C. V. Pagba, **H. Hwang**, **J. C. Gumbart**, S.-H. Chi, J. W. Perry, and B. A. Barry. *Chem. Commun*. 55:9399-9402, 2019.

75*. Stable calcium-free myocilin olfactomedin domain variants reveal challenges in differentiating between benign and glaucoma-causing mutations. S. E. Hill, M. S. Kwon, M. D. Martin, A. Suntharalingam, **A. Hazel**, C. A. Dickey, **J. C. Gumbart**, and R. L. Lieberman. *J. Biological Chemistry*. 294:12717-12728, 2019.

74*. Accelerating membrane simulations with Hydrogen Mass Repartitioning. **C. Balusek, H. Hwang**, C.H. Lau, **K. Lundquist, A. Hazel, A. Pavlova**, D.L. Lynch, P.H. Reggio, Y. Wang, and **J.C. Gumbart***. *J. Chemical Theory and Computation*. 15:4673-4686, 2019.

73*. A Novel Human IL2RB Mutation Results in T and NK cell-driven Immune Dysregulation. I. Z. Fernandez, R. M. Baxter, J. E. Garcia-Perez, E. Vendrame, T. Ranganath, D.S. Kong, **K. Lundquist**, T. Nguyen, S. Ogolla, J. Black, C. Galambos, **J.C. Gumbart**, N. Dawany, J.R. Kelsen, E.F. De Zoeten, R. Quinones, H. Eissa, M. Verneris, K. E. Sullivan, R. Rochford, C.A. Blish, R.M. Kedl, C.M. Dutmer, and E.W.Y. Hsieh. *J. Experimental Medicine.* 216:1255-1267, 2019.

72*. ATP-dependent signaling in simulations of a revised model of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). K.M. Strickland, **G. Stock**, G. Cui, **H. Hwang**, D.T. Infield, I. Schmidt-Krey, N.A. McCarty, and **J.C. Gumbart***. *J. Physical Chemistry B.* 123:3177-3188, 2019.

71*. The structure and function of tryptophan-tyrosine dyads in biomimetic β hairpins. T. McCaslin, C. V Pagba, S.-H. Chi, **H. Hwang**, **J. C. Gumbart**, J. Perry, C. Olivieri, F. Porcelli, G. Veglia, Z. Guo, M. McDaniel, B. A. Barry. *J. Physical Chemistry B*. 123:2780-2791, 2019.

70*. Identification of Binding Sites for Efflux Pump Inhibitors of the *Escherichia coli* AcrAB-TolC component AcrA. Z. Darzynkiewicz, A. Green, N. Abdali, **A. Hazel**, R. Fulton, J. Kimball, Z. Gryczynski, **J.C. Gumbart**, J. Parks, J. Smith, H. Zgurskaya. *Biophysical Journal.* 116:648-658, 2019.

69*. Transmembrane But Not Soluble Helices Fold Far Inside the Ribosome tunnel. M. Bañó-Polo, C. Baeza-Delgado, S. Tamborero, **A. Hazel**, I. Nilsson, P. Whitley, **J. C. Gumbart**, G. von Heijne, I. Mingarro. *Nature Communications.* 9:5246, 2018.

68*. Distribution of mechanical stress in the *Escherichia coli* cell envelope. **H. Hwang**, N. Paracini, J. M. Parks, J. H. Lakey, and **J. C. Gumbart***. *Biochimica et Biophysica Acta (BBA) – Biomembranes*. 1860:2566-2575, 2018.

67*. Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. **Y. Wang**, J. Comer, Z. Chen, J. Chen, and **J. C. Gumbart***. *Environmental Science: Nano*. 5:2117-2128, 2018.

66*. C-terminal kink formation is required for lateral gating in BamA. **K. Lundquist**, J. Bakelar, N. Noinaj, and **J.C. Gumbart***. *Proceedings of the National Academy of Sciences, USA*, 115:E7942-E7949, 2018.

65*. Folding free energy landscapes of β-sheets with non-polarizable and polarizable CHARMM force fields. **A. Hazel**, E. T. Waters, C. N. Rowley, **J. C. Gumbart***. *J. Chemical Physics*. 149:072317, 2018.

64*. Computed free energies of peptide insertion into bilayers are independent of computational method. **J. C. Gumbart***, M. Ulmschneider, **A. Hazel**, S. H. White, and J. Ulmschneider*. *J. Membrane Biology*. 251:345-456, 2018.

63*. BFEE: A user-friendly graphical interface facilitating absolute binding free-energy calculations. H. Fu, **J.C. Gumbart**, H. Chen, X. Shao, W. Cai, and C. Chipot. *J. Chemical Information and Modeling*. 58:556-560, 2018.

62*. Development of CHARMM-compatible force-field parameters for cobalamin and related cofactors from quantum mechanical calculations. **A. Pavlova**, J.M. Parks*, and **J.C. Gumbart***. *J. Chemical Theory and Computation*. 14:784-798, 2018.

61*. Producing membrane proteins one simulation at a time. **J.C. Gumbart***. *J. Biological Chemistry*. 292:19546-19547, 2017.

60*. Structure and misfolding of the flexible tripartite coiled coil domain of glaucoma-associated myocilin. S. E. Hill, E. Nguyen, R. K. Donegan, **A. Hazel**, **J.C. Gumbart**, and R. L. Lieberman. *Structure*. 25:1697-1707, 2017.

59*. Structural basis for substrate selection by the translocation and assembly module of the beta-barrel assembly machinery. R.S. Bamert[1], **K. Lundquist[1], H. Hwang[1]**, C.T. Webb, T. Shiota, C.J. Stubenrauch, M.J. Belousof, R.J.A. Goode, R.B. Schittenhelm, R. Zimmerman, M. Jung**, J.C. Gumbart***, and T. Lithgow*. *Molecular Microbiology*. 106:142-156, 2017. [1]Co-first authors.

58*. Toward the rational design of macrolide antibiotics to combat resistance. **A. Pavlova**, J.M. Parks, A.K. Oyelere, **J.C. Gumbart***. *Chemical Biology & Drug Design*. 90:641-652, 2017.

57*. Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired β-Hairpin Maquette Determined through Spectroscopy and Simulation. **H. Hwang**, T. McCaslin, **A. Hazel**, C. Pagba, C. Nevin, **A. Pavlova**, B. Barry*, **J.C. Gumbart***. *J. Physical Chemistry B*. 121:3536-3545, 2017.

56*. The β-barrel assembly machinery in motion. N. Noinaj, **J.C. Gumbart**, and S. Buchanan. *Nature Reviews Microbiology*. 15:197-204, 2017.

55*. Role of the native outer-membrane environment on the transporter BtuB. **C. Balusek** and **J.C. Gumbart***. *Biophysical Journal*. 111:1409-1417, 2016.

54. Dynamic behavior of Trigger Factor on the ribosome. J. Deeng, K.Y. Chan, E.O. van der Sluis, L. Bischoff, O. Berninghausen, W. Han, **J.C. Gumbart**, K. Schulten, B. Beatrix and R. Beckmann. *J. Molecular Biology*. 428:3588-3602, 2016.

53*. Transitions of Double-Stranded DNA Between the A- and B-Forms. J. T. Waters, X.-J. Lu, R. Galindo-Murillo, **J.C. Gumbart**, H.D. Kim, T.E. Cheatham III, and S.C. Harvey. *J. Physical Chemistry B*. 120:8449-8456, 2016.

52*. DNA Scrunching in the Packaging of Viral Genomes. J.T. Waters, H.D. Kim, **J.C. Gumbart**, X.-J. Lu, and S.C. Harvey. *J. Physical Chemistry B*. 120:6200-6207, 2016.

51*. Simulation-based approaches for determining membrane permeability of small compounds. C. Lee, J. Comer, **C. Herndon** @, N. Leung, **A. Pavlova**, R. Swift, C. Tung, C. Rowley, R. Amaro, C. Chipot, Y. Wang, and **J.C. Gumbart***. *J. Chemical Information and Modeling*. 56:721-733, 2016.

50*. Structural and Functional Characterization of the LPS Transporter LptDE from Gram-negative Pathogens. I Botos, N. Majdalani, S.J. Mayclin, J.G. McCarthy, **K. Lundquist**, D. Wojtowicz, T.J. Barnard, **J.C. Gumbart**, and S. K. Buchanan. *Structure*. 24:965-976, 2016.

49*. Membrane proteins: Where theory meets experiment. J.C. Gumbart and S. Noskov. *BBA – Biomembranes*. 1858:1553-1555, 2016.

48*. Decrypting protein insertion through the translocon with free-energy calculations. **J.C. Gumbart*** and C. Chipot. *BBA – Biomembranes*. 1858:1663-1671, 2016.

47*. Living on the edge: Simulations of bacterial outer-membrane proteins. **A. Pavlova, H. Hwang, K. Lundquist, C. Balusek,** and **J.C. Gumbart***. *BBA – Biomembranes*. 1858:1753-1759, 2016.

46*. Accelerating the use of molecular modeling in the high school classroom with VMD lite. **K. Lundquist**, **C. Herndon** @, T.H. Harty, and **J.C. Gumbart***. *Biochemistry and Molecular Biology Education*. 44:124-129, 2016.

45*. Parametrization of macrolide antibiotics using the Force Field Toolkit. **A. Pavlova** and **J.C. Gumbart***. *J. Computational Chemistry*. 36:2052-2063, 2015.

44*. Coarse-grained simulations of bacterial cell wall growth reveal that local coordination alone can be sufficient to maintain rod shape. L.T. Nguyen, **J.C. Gumbart**, M. Beeby, and G.J. Jensen. *Proceedings of the National Academy of Sciences, USA*. 112:E3689-E3698, 2015.

43*. Conformational changes of the clamp of the protein translocation ATPase SecA. Y. Chen, B.W. Bauer, T.A. Rapoport, and **J.C. Gumbart***. *J. Molecular Biology*. 427:2348-2359, 2015.

42*. Structural and biophysical characterization of epitope-specific engineered Fab fragment and complexation with membrane proteins: implications for co-crystallization. J. L. Johnson, K. C. Entzminger, J. Hyun, S. Kalyoncu, D.P. Heaner, I.A. Morales, A. Sheppard, **J.C. Gumbart**, J.A. Maynard and R.L. Lieberman. *Acta Crystallographica D*. 71:896-906, 2015.

41*. The Adaptive Biasing Force method: Everything you always wanted to know, but were afraid to ask. J. Comer, **J.C. Gumbart**, J. Hénin, T. Lelièvre, A. Pohorille, and C. Chipot. *J. Physical Chemistry B*. 119:1129-1151. 2015.

40*. Lateral opening and exit pore formation are required for BamA function. N. Noinaj, A.J.

Kuszak, **C. Balusek**, **J.C. Gumbart**, and S.K. Buchanan. *Structure*. 22:1055-1062, 2014.

39*. Thermodynamics of deca-alanine folding in water. **A. Hazel**, C. Chipot, and **J.C. Gumbart***. *J. Chemical Theory and Computation*. 10:2836-2844, 2014.

38*. *Escherichia coli* peptidoglycan structure and mechanics as predicted by atomic-scale simulations. **J.C. Gumbart***, M. Beeby, G.J. Jensen, and B. Roux. *PLoS Computational Biology*. 10:e1003475, 2014.

37*. Structure of the SecY channel during initiation of protein translocation. E. Park, J.F. Menetret, **J.C. Gumbart**, S.J. Ludtke, W. Li, A. Whynot, T.A. Rapoport, and C.W. Akey. *Nature*. 506:102-106, 2014.

36. Generalized Scalable Multiple Copy Algorithms for Molecular Dynamics Simulations in NAMD. W. Jiang, J. Phillips, L. Huang, M. Fajer, Y. Meng, **J.C. Gumbart**, Y. Luo, K. Schulten, and B. Roux. *Computer Physics Communications*. 185:908-916, 2014.

35*. The mechanism of the amidases: Mutating the glutamate adjacent to the catalytic triad inactivates the enzyme due to substrate mispositioning. B.W. Weber, S.W. Kimani, A. Varsani, D.A. Cowan, R. Hunter, G.A. Venter, **J.C. Gumbart**, B.T. Sewell. *J. Biological Chemistry*. 288:28514-28523, 2013.

34. Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. F. Khalili-Araghi, B. Ziervogel, **J.C. Gumbart**, and B. Roux. *J. General Physiology*. 142:365-475, 2013.

33*. Rapid parameterization of small molecules using the Force Field Toolkit. C.G. Mayne, J. Saam, K. Schulten, E. Tajkhorshid, and **J.C. Gumbart***. *J. Computational Chemistry*. 34:2757-2770, 2013.

32. Efficient determination of protein-protein standard binding free energies from first principles. **J.C. Gumbart**, B. Roux, and C. Chipot. *J. Chemical Theory and Computation*. 9:3789-3798, 2013.

31*. Structural insight into the biogenesis of β-barrel membrane proteins. N. Noinaj, A.J. Kuszak, **J.C. Gumbart**, P. Lukacik, H. Chang, N. Easley, T. Lithgow, and S.K. Buchanan. *Nature*. 501:385-390, 2013.

30. The mobility of two kinase domains in the *Escherichia coli* chemoreceptor array varies with signaling state. A. Briegel, P. Ames, **J.C. Gumbart**, C.M. Oikonomou, J.S.Parkinson, and G.J. Jensen. *Molecular Microbiology*. 89:831-841, 2013.

29. IcmQ in the type 4b secretion system contains an NAD^+ binding domain. J.D. Farelli, **J.C. Gumbart**, I.V. Akey, A. Hempstead, W. Amyot, J.F. Head, C.J. McKnight, R.R. Isberg, and C.W. Akey. *Structure*. 21:1361-1373, 2013.

28. Architecture and assembly of the Gram-positive cell wall. M. Beeby, **J.C. Gumbart**, B. Roux, and G.J. Jensen. *Molecular Microbiology*, 88:664-672, 2013.

27. Reconciling the roles of kinetic and thermodynamic factors in membrane-protein insertion. **J.C. Gumbart**, I. Teo, B. Roux, and K. Schulten. *J. American Chemical Society*. 135:2291-2297, 2013.

26. Standard binding free energies from computer simulations: What is the best strategy? **J.C. Gumbart**, B. Roux, and C. Chipot. *J. Chemical Theory and Computation*, 9:794-802, 2013.

25. A new crystal form of MshB from *Mycobacterium tuberculosis* with glycerol and acetate in

the active site suggests the catalytic mechanism. S.G. Broadley, **J.C. Gumbart**, B.W. Weber, M.J. Marakalala, D.J. Steenkamp, and B.T. Sewell. *Acta Cryst. D*, 68:1450-1459, 2012.

24. Mechanisms of SecM-mediated stalling in the ribosome. **J. Gumbart**, E. Schreiner, D.N. Wilson, R. Beckmann, and K. Schulten. *Biophys. J.*, 103:331-341, 2012.

23. Determination of membrane-insertion free energies by molecular dynamics simulations. **J. Gumbart** and B. Roux. *Biophys. J.*, 104:795-801, 2012.

22. Structural basis for iron piracy by pathogenic *Neisseria.* N. Noinaj, N.C. Easley, M. Oke, N. Mizuno, **J. Gumbart**, E. Boura, A.N. Steere, O. Zak, P. Aisen, E. Tajkhorshid, R.W. Evans, A.R. Gorringe, A.B. Mason, A.C. Steven, and S.K. Buchanan. *Nature*, 483:53-58, 2012.

21. Molecular basis for activation of a catalytic asparagine residue in a self-cleaving bacterial autotransporter. T.J. Barnard, **J. Gumbart**, J.H. Peterson, N. Noinaj, N.C. Easley, N. Dautin, A. J. Kuszak, E. Tajkhorshid, H.D. Bernstein, and S.K. Buchanan. *J. Molecular Biology,* 415:128-142, 2012.

20. Constant electric field simulations of the membrane potential illustrated with simple systems. **J. Gumbart**, F. Khalili-Araghi, M. Sotomayor, and B. Roux. *BBA – Biomembranes*, 1818:294-302, 2012.

19. Symmetry-restrained flexible fitting for symmetric EM maps. K.-Y. Chan, **J. Gumbart**, R. McGreevy, J.M. Watermeyer, B.T. Sewell, and K. Schulten. *Structure*, 19:1211-1218, 2011.

18. Free energy of nascent-chain folding in the translocon. **J. Gumbart**, C. Chipot, and K. Schulten. *J. American Chemical Society*, 133:7602-7607, 2011.

17. Cryo-EM structure of the ribosome-SecYE complex in the membrane environment. J. Frauenfeld, **J. Gumbart**, E.O. van der Sluis, S. Funes, M. Gartmann, B. Beatrix, T. Mielke, O. Berninghausen, T. Becker, K. Schulten, and R. Beckmann. *Nature Structural and Molecular Biology,* 18:614-621, 2011.

16. Free-energy cost for translocon-assisted insertion of membrane proteins. **J. Gumbart**, C. Chipot, and K. Schulten. *Proceedings of the National Academy of Sciences, USA*, 108:3596-3601, 2011.

15. Applications of the molecular dynamics flexible fitting method. L.G. Trabuco, E. Schreiner, **J. Gumbart**, J. Hsin, E. Villa, and K. Schulten. *J. Structural Biology*, 173:420-427, 2011.

14. Self-assembly of photosynthetic membranes. J. Hsin, D. Chandler, **J. Gumbart**, C.B. Harrison, M. Sener, J. Strumpfer, and K. Schulten. *ChemPhysChem*, 11:1154-1159, 2010.

13. Structure of monomeric yeast and mammalian Sec61 complexes interacting with the translating ribosome. T. Becker, E. Mandon, S. Bhushan, A. Jarasch, J.-P. Armache, S. Funes, F. Jossinet, **J. Gumbart**, T. Mielke, O. Berninghausen, K. Schulten, E. Westhof, R. Gilmore, and R. Beckmann. *Science*, 326:1369-1373, 2009.

12. Membrane curvature induced by aggregates of LH2s and monomeric LH1s. D. Chandler, **J. Gumbart**, J.D. Stack, C. Chipot, and K. Schulten. *Biophys. J.*, 97:2978-2984, 2009.

11. Regulation of the protein-conducting channel by a bound ribosome. **J. Gumbart**, L.G. Trabuco, E. Schreiner, E. Villa, and K. Schulten. *Structure*, 17:1453-1464, 2009.

10. Coupling of calcium and substrate binding through loop alignment in the outer membrane transporter BtuB. **J. Gumbart**, M.C. Wiener, and E. Tajkhorshid. *J. Molecular Biology*, 393:1129-1142, 2009.

9. Protein-induced membrane curvature investigated through molecular dynamics flexible fitting. J. Hsin, **J. Gumbart**, L.G. Trabuco, E. Villa, P. Qian, C.N. Hunter, and K. Schulten. *Biophys. J.*, 97:321-329, 2009.

8. Molecular dynamics simulations of membrane channels and transporters. F. Khalili-Araghi, **J. Gumbart**, P.-C. Wen, M. Sotomayor, E. Tajkhorshid, and K. Schulten. *Current Opinion in Structural Biology*, 19:128-137, 2009.

7. The roles of pore ring and plug in the SecY protein-conducting channel. **J. Gumbart** and K. Schulten. *J. General Physiology*, 132:709-719, 2008.

6. Intrinsic curvature properties of photosynthetic proteins in chromatophores. D. Chandler, J. Hsin, C.B. Harrison, **J. Gumbart**, and K. Schulten. *Biophys. J.*, 95:2822-2836, 2008.

5. Structural determinants of lateral gate opening in the protein translocon. **J. Gumbart** and K. Schulten. *Biochemistry*, 46:11147-11157, 2007.

4. Mechanics of force propagation in TonB-dependent outer membrane transport. **J. Gumbart**, M.C. Wiener, and E. Tajkhorshid. *Biophys. J.*, 93:496-504, 2007.

3. Molecular dynamics studies of the archaeal translocon. **J. Gumbart** and K. Schulten. *Biophys. J.*, 90:2356-2367, 2006.

2. Scalable molecular dynamics with NAMD. J.C. Phillips, R. Braun, W. Wang, **J. Gumbart**, E. Tajkhorshid, E. Villa, C. Chipot, R.D. Skeel, L. Kale, and K. Schulten. *J. Computational Chemistry*, 26:1781-1802, 2005.

1. Molecular dynamics simulations of proteins in lipid bilayers. **J. Gumbart**, Y. Wang, A. Aksimentiev, E. Tajkhorshid, and K. Schulten. *Current Opinion in Structural Biology*, 15:423-431, 2005.

B2. Conference Presentations with Proceedings

1. Long time and large size molecular dynamics simulations made feasible through new Teragrid hardware and software. K. Vandivort, J.C. Phillips, E. Villa, P.L. Freddolino, **J. Gumbart**, L. G. Trabuco, D.E. Chandler, J. Hsin, C.B. Harrison, L. Kale, and K. Schulten. *Proceedings of the 2008 TeraGrid Conference*, 2008.

C. Other Publications and Creative Products

Tutorials: these serve to guide readers in the application of various computational methods

1. Protein:ligand standard binding free energies. Last update Sept. 2017 co-author: C. Chipot
2. Forcing substrates through channels. Last update Sept. 2017 co-author: A. Hazel (graduate student, Physics)
3. Adaptive biasing force calculations in NAMD. Last update Sept. 2017 co-authors: C. Chipot, J. Henin
4. Alchemical free energy perturbation calculations. Last update Sept. 2017 co-authors: C. Chipot, J. Henin

Case studies: these present an exploration of scientific topics using molecular visualization software

1. (2011) Light Harvesting Complex 2 co-authors: D. Chandler, J. Hsin
2. (2006) Ubiquitin co-authors: E. Cruz-Chu

D. Presentations

Invited presentations at conferences:

27) July 2019: Adaptation of the *Escherichia coli* cell envelope to mechanical stress. International Physics of Living Systems meeting. Max Planck Institute for Biochemistry, Munich, Germany.

26) June 2019: Adaptation of the *Escherichia coli* cell envelope to mechanical stress. Bacterial Cell Envelope: New insights into structure and antimicrobial targets. Rocky Mountain Laboratory, Hamilton, MT.

25) June 2019: Conformational dynamics of AcrA govern multidrug efflux pump assembly. Free energy calculations: Entering the fourth decade of adventure in chemistry and biophysics. Santa Fe, NM.

24) June 2019: Distribution of mechanical stress in the *E. coli* cell envelope. Biological membranes and membrane proteins: Challenges for theory and experiment. Santa Fe, NM.

23) August 2018: Flexibility of free and bound AcrA in the AcrAB-TolC multidrug efflux pump of *E. coli* determined using 3D PMFs. American Chemical Society National Meeting. Boston, MA.

22) June 2018: Complex dynamics in the BAM outer-membrane-protein insertion machinery. FASEB meeting on Molecular Biophysics of Membranes. Olean, NY.

21) May 2018: Conformational dynamics of HBV capsid proteins in free and drug-bound states. Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design. Cambridge, MA.

20) Nov. 2017: Over a decade of studying membrane-protein insertion. Klaus Schulten Memorial Symposium. Urbana, IL.

19) July 2017: Folding and inserting outer-membrane porins. Transport mechanisms in biological and synthetic nanopores and channels. Bremen, Germany.

18) July 2017: Protein folding in the bacterial cell envelope. Free energy calculations: Three decades of adventure in chemistry and biophysics. Telluride, CO.

17) June 2017: Elastic properties of the Gram-negative cell envelope. Biological membranes and membrane proteins: Challenges for theory and experiment. Santa Fe, NM.

16) June 2017: Estimating small-molecule permeability from membrane deformation**.** CECAM workshop - Beyond Kd's: New computational methods to address challenges in drug discovery. Lausanne, Switzerland.

15) May 2017: Protein folding at the bacterial outer membrane. Biophysics 2017 Mexico City. Mexico City, Mexico.

14) June 2016: Pathway- and Environment-dependent Protein Folding Energetics. Canadian Chemistry Conference and Exhibition. Halifax, NS, Canada.

13) May 2016: MD-guided design of new inhibitors against Hepatitis B Virus. Workshop on Free Energy Methods in Drug Design: Targeting Cancer. Boston, MA.

12) Mar. 2016: Details matter! Building the outer membranes of Gram-negative bacteria. Frontiers in Structural Biology of Membrane Proteins. Huntsville, AL.

11) Nov. 2015: Bridging the gap between X-ray crystallography and biological insight with MD simulations. The 25th Hot Spring Harbor International Symposium. Fukuoka, Japan.

10) July 2015: Adaptive Biasing Forces (ABF): A love-hate relationship. Free-energy calculations: A mathematical perspective. Oaxaca, Mexico.

9) July 2015: Simulating the periplasmic space of Gram-negative bacteria. Translocation Workshop on the Molecular basis of antibiotic permeability in Gram-negative bacteria. Bremen, Germany.

8) June 2015: Simulating the periplasm of Gram-negative bacteria. Workshop on Challenges in Large-Scale Biomolecular Simulations. Telluride, CO.

7) Oct. 2014: A computational glimpse into the peculiar properties of bacterial outer-membrane proteins. Memorial University Biophysics Symposium. St. John's, Newfoundland, Canada.

6) July 2014: Exploring the complex free energy landscape of helix formation. Gordon Research Conference on Computational Chemistry. Mount Snow, VT.

5) May 2014: Converging on an accurate description of water-membrane partitioning. Workshop on Free Energy Methods in Drug Design. Boston, MA.

4) Jan. 2014: Single-molecule views of membrane-protein insertion from MD simulations. XVI Annual Linz Winter Workshop. Linz, Austria.

3) Dec. 2013: Outer-membrane protein assembly and insertion. Atlanta-Area Molecular and Cellular Biophysics Symposium. Atlanta, GA.

2) July 2013: Membrane-protein insertion at two membranes: Analogous mechanisms at work? Biological membranes and membrane proteins: Challenges for theory and experiment. Snowmass, CO.

1) July 2013: Partitioning of small helices in membranes: A story of two force fields. Free energy calculations: Three decades of adventure in chemistry and biophysics. Snowmass, CO.

prior to starting at GT

6) Sept. 2012: Engineering the bacterial cell wall. CPLC Symposium. Urbana, IL.

5) July 2012: Application of free-energy methods in NAMD to complex biological systems. CECAM Workshop on Free energy calculations: From theory to applications, 2012. Paris, France.

4) Aug. 2011: Determining structures of membrane proteins through combined cryo-electron microscopy and molecular dynamics. Synthetic Biology International Workshop, UC Berkeley. Berkeley, CA.

3) July 2011: Protein localization and folding mechanisms revealed by molecular dynamics simulations. South African Institute of Physics Conference. Pretoria, South Africa.

2) July 2011: Computational microscopy using molecular dynamics. Biophysics Workshop, South African Institute of Physics Conference. Pretoria, South Africa.

1) Sept. 2008: Membrane protein insertion in the translocon. CECAM Workshop on Membrane Protein Insertion: Theory and Experiment. Lausanne, Switzerland.

<u>Invited presentations at universities & institutes:</u>

24) September 2019: The "when" and "where" of protein folding. Georgia State University, Atlanta, GA.

23) June 2019: Conformational dynamics of AcrA govern multidrug efflux pump assembly. Center for Nonlinear Sciences, Los Alamos National Lab. Los Alamos, NM.

22) April 2019: A glimpse inside the cell with a computational microscope. Physics Field Day, Georgia Tech. Atlanta, GA.

21) Oct. 2018: Engineering the bacterial cell envelope. University of Vermont, Burlington, VT.

20) Mar. 2018: Designer drugs from basic physics. Society of Physics Students, Georgia Tech. Atlanta, GA.

19) Jan. 2018: Molecular mechanisms of nutrient acquisition and virulence revealed by MD simulations. 2018 Suddath Symposium. Georgia Tech. Atlanta, GA.

18) Dec. 2017: A physicist's perspective on drug design: Insights from molecular dynamics simulations. Wichita State Univ. Wichita, KS.

17) Mar. 2017: Lessons on β-sheet folding from bacteria and from MD simulations. Florida State Univ. Tallahassee, FL.

16) Nov. 2016: Inside-out and outside-in: breaking into the bacterial outer membrane. Purdue Univ. West Lafayette, IN.

15) Aug. 2016: Inside-Out and Outside-In: Breaking Through the Bacterial Outer Membrane. U. Arkansas. Fayetteville, AR.

14) Apr. 2016: Details Matter! Building the Outer Membranes of Gram-Negative Bacteria One Atom at a Time. U. Michigan. Ann Arbor, MI.

13) Mar. 2016: Details Matter! Building the Outer Membranes of Gram-Negative Bacteria One Atom at a Time. Clark Atlanta U. Atlanta, GA.

12) Nov. 2015: Simulating the periplasmic space of Gram-negative bacteria. RIKEN Institute. Tokyo, Japan.

11) Oct. 2015: Simulating the periplasmic space of Gram-negative bacteria. U. Tennessee, Knoxville. Knoxville, TN.

10) Sept. 2015: Simulating the periplasmic space of Gram-negative bacteria. Ohio State University. Columbus, OH.

9) Jan. 2015: Barreling through the outer membrane one protein at a time. Universidad Andrés Bello. Santiago, Chile.

8) Oct. 2014: Barreling through the outer membrane one protein at a time. Oak Ridge National Laboratory. Oak Ridge, TN.

7) Aug. 2014: Addressing the arduous problem of calculating free energies of biological processes. Physics Dept. seminar, Chinese University of Hong Kong. Hong Kong, China.

6) May 2014: A computational glimpse into the peculiar properties of bacterial outer-membrane proteins. Biochemistry Department Seminar, Emory University. Atlanta, GA.

5) Oct. 2013: Assembly and architecture of Gram-positive and –negative cell walls. Biology Department Seminar, Georgia Tech. Atlanta, GA.

4) Oct. 2013: Bringing physics to life or: How I learned to stop worrying and love biology. Society of Physics Students, Georgia Tech. Atlanta, GA.

3) Aug. 2013: Mechanisms of membrane-protein insertion at the inner and outer membranes. Molecular Biophysics Research Review, Georgia Tech. Atlanta, GA.

2) May 2013: A molecular balancing act: the coupled roles of energetics and kinetics in the insertion of membrane proteins. Physics Dept. Colloquium, Emory University, Atlanta, GA.

1) Apr. 2013: Mechanisms of SecM-mediated stalling in the ribosome. RiboEvo Seminar, Georgia Tech. Atlanta, GA.

prior to starting at GT

11) Dec. 2012: Stalling of the ribosome by SecM. Mankin Lab group meeting, UIC. Chicago, IL.

10) Oct. 2012: Bringing physics to life or: How I learned to stop worrying and love biology. Graduate student seminar series, Georgia Tech. Atlanta, GA.

9) March 2012: Glimpsing the inner workings of living cells with the computational microscope. Argonne National Laboratory. Argonne, IL.

8) March 2012: Membrane-protein insertion: One helix and one amino acid at a time. Physics Dept. seminar, IUPUI. Indianapolis, IN.

7) March 2012: Membrane-protein insertion: One helix and one amino acid at a time. Physics Dept. seminar, Georgia Tech. Atlanta, GA.

6) Jan. 2012: Membrane-protein insertion: One helix and one residue at a time. Chemistry Dept. seminar, Washington University. St. Louis, MO.

5) Oct. 2011: Membrane protein folding and insertion mediated by the Sec translocon. Beckmann Lab group meeting, U. Munich. Munich, Germany.

4) Aug. 2011: Development and function of proteins in the inner and outer membranes. Jensen Lab group meeting, Caltech. Pasadena, CA.

3) March 2011: Realizing Feynman's dream with the computational microscope. James Gumbart. Western Illinois Univ. Physics Dept. colloquium. Macomb, IL.

2) March 2011: Directing protein traffic across, and into, membranes. Buchanan Lab group meeting, NIH. Bethesda, MD.

1) March 2008: Bringing physics to life: Biological insights from computer simulations. James Gumbart. Western Illinois Univ. Physics Dept. colloquium. Macomb, IL.

<u>Contributed presentations at conferences:</u>

5) July 2019: Adaptation of the *Escherichia coli* cell envelope to mechanical stress. International Physics of Living Systems Network meeting. Munich, Germany.

4) June 2018: Hydrogen-mass repartitioning in NAMD. NAMD Developer Workshop. Urbana, IL.

3) May 2017: Using REST2 in NAMD: Is it worth it? NAMD Developer Workshop. Chicago, IL.

2) July 2016: Structure and mechanics of the bacterial cell wall. iPoLS 2016 Network Meeting at Harvard. Cambridge, MA.

1) July 2016: Simulations of BamA in a native outer-membrane model and energetics of lateral opening. FASEB meeting on Molecular Biophysics of Membranes. Snowmass, CO.

prior to starting at GT

5) Feb. 2012: Spontaneous movement of transmembrane segments from SecY into the membrane. Biophysical Society Annual Meeting. San Diego, CA.

4) July 2011: Reproduction of experimental free energies of membrane insertion using molecular dynamics. Biological Membranes and Membrane Proteins Conference. Snowmass, CO.

3) Feb. 2010: The role of the protein-conducting channel in the membrane insertion of transmembrane segments. Biophysical Society Annual Meeting. San Francisco, CA.

2) Feb. 2009: Regulation of the protein-conducting channel by a bound ribosome. Biophysical Society Annual Meeting. Boston, MA.

1) Feb. 2007: Mechanics of force propagation in TonB-dependent outer membrane transporters. Biophysical Society Annual Meeting. Baltimore, MD.

E. Grants and Contracts

E1. As Principal Investigator

Currently funded:

09/2017 – 06/2022 NIH R01-GM123169 $1,400,398 total ($1,011,687 direct) PI
Dynamic characterization of outer-membrane-protein biogenesis by the BAM and TAM complexes

06/2015 – 05/2020 NSF MCB-1452464 $795,554 total ($584,770 direct) PI
CAREER: Research and education on protein folding as an energy source at the bacterial outer membrane

10/2018 – 09/2019 NSF XRAC MCB130173 9.72 million CPU-hours PI
Structure and dynamics of bacteria-specific systems
XRAC is a part of NSF that awards time on national supercomputers. The current award represents an investment of $120,613 according to NSF.

Previous funding:

10/2017 – 09/2018 NSF XRAC MCB130173 8.93 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

01/2017 – 12/2017 DOE INCITE 38 million CPU-hours PI
Determining the role of AcrA in the bacterial multidrug efflux pump
Co-Investigators: Jerome Baudry (U. Tennessee, Knoxville) and Jerry Parks (ORNL)
DOE's INCITE program provides computational time on one of the fastest supercomputers in the world. This project was one of only four selected in the field of biophysics.

10/2016 – 09/2017 NSF XRAC MCB130173 9.59 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

10/2015 – 09/2016 NSF XRAC MCB130173 15.48 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

05/2013 – 05/2016 NIH K22-AI100927 $268,585 total ($250,000 direct) PI
Combating infection through atomic-scale modeling of unique bacterial systems

05/2014 – 12/2015 BWF Travel Award $9,950 total PI
Development of novel approaches and models for permeability calculations

11/2014 – 10/2015 Anton PSCA14044P 100,000 CPU-hours PI
Determining the mechanisms of protein folding in membranes
Anton is a special-purpose supercomputer developed by DE Shaw Research. The only one publically available is housed at Pittsburgh Supercomputing Center. The award of 100,000

hours is the maximum possible and represents over 2% of the machine's entire annual capability.

10/2014 – 09/2015 NSF XRAC MCB130173 6.92 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

11/2013 – 10/2014 Anton PSCA13032P 100,000 CPU-hours PI
Determining the mechanisms of protein folding in membranes

10/2013 – 09/2014 NSF XRAC MCB130173 6.5 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

11/2012 – 10/2013 Anton PSCA12028P 100,000 CPU-hours PI
Determining the mechanisms of protein folding in membranes

E2. As Co-Principal Investigator

Currently funded:

09/2018 – 08/2023 NSF PHY-1806833 $2,400,000 total Co-PI
Collaborative Research: Formation of a High Flux Student Research Network

Previous funding:

04/2013 – 03/2018 NIH R01-GM101425 $113,000 direct to JCG Co-I
Structural basis of chemoreception PI: Grant Jensen (Caltech)

07/2015 – 06/2016 NSF XRAC MCB150053 787,000 CPU-hours Co-PI
Computational Investigation of DNA Packaging Motors in Bacteriophages:
The Scrunchworm Hypothesis PI: Stephen Harvey (Univ. of Pennsylvania)

07/2013 – 06/2015 NIH R01-GM067887 $123,000 direct to JCG Co-I
Mechanisms of membrane proteins through in-situ modeling. PI: Klaus Schulten (UIUC)

F. Other Scholarly Accomplishments

Software development

2013 – current: Force field toolkit (FFTK), a plugin to the molecular visualization program VMD that aids users in developing novel simulation parameters for small molecules. The source paper (#33 above) has 195 citations in five years.

2014 – current: VMD lite, a plugin for the molecular visualization program VMD that provides a GUI interface simplifying many features. It is used in education, and specific lesson modules have been and are continuing to be created for it on topics such as membranes and ATP hydrolysis.

V. Teaching

A. Courses Taught

Fall 2019	Physics 4251/6250	Biophysics	18 students
Spring 2019	Physics 4601	Senior Seminar I	50 students
Spring 2019	Physics 2212	Intro Physics of Living Systems II	54 students
Fall 2018	Physics 4251/8803	Biophysics	11 students
Spring 2018	Physics 4601	Senior Seminar I	48 students
Spring 2018	Physics 2212	Intro Physics of Living Systems II	71 students
Fall 2017	Physics 4251/8803	Biophysics	15 students
Spring 2017	Physics 4601	Senior Seminar I	14 students
Spring 2017	Physics 2212	Intro Physics of Living Systems II	50 students

Developed course from scratch with Jennifer Curtis, who taught the first semester.

Fall 2016	Physics 4601	Senior Seminar I	40 students
Spring 2016	Physics 4251/8803	Biophysics	14 students
Fall 2015	Physics 4601	Senior Seminar I	24 students

Took over and redeveloped course from scratch to focus on GRE subject test preparation, graduate school applications, and careers outside of academia.

Fall 2015	Physics 2211	Intro Physics I	170 students
Fall 2014	Physics 4251/8803	Biophysics	11 students
Fall 2013	Physics 4251/8803	Biophysics	10 students

B. Individual Student Guidance

B1. PhD Students

8. Katie Kuo	GT Chemistry	Oct. 2018 – current
7. Zijian Zhang	GT Physics	Dec. 2017 – current
6. David Ryoo	GT Bioengineering	Oct. 2017 – current
5. Yui Tik Pang	GT Physics	Aug. 2017 – current
4. Hyea Hwang	GT Materials Science & Eng.	Dec. 2014 – Jan. 2019 *Defended 12/2018*

DOE SCSGR Award recipient to work at Oak Ridge National Lab (11/2017-7/2018)

3. Karl Lundquist	GT Physics	Jan. 2014 – Jan. 2019 *Defended 12/2018*

GAANN fellowship recipient Aug. 2013 – Aug. 2015

2. Anthony Hazel	GT Physics	Apr. 2013 – Jan. 2019 *Defended 12/2018*

Larry S. O'Hara Fellowship Jan. 2017 – Dec. 2017

1. Curtis Balusek	GT Physics	Jan. 2013 – Jan. 2019 *Defended 12/2018*

GAANN fellowship recipient, Aug. 2013 – Aug. 2015
Bonnie B. and Charles K Rice Jr. Fellowship, Aug. 2015 – Aug. 2016
School of Physics TA of the Year Award 2016, 2017
Biophysical Society Meeting Education Committee Travel Award Winner, Feb. 2017

B2. M.S. students

3. Gorman Stock	M.S. non-thesis	GT Chemistry	Jan. 2014 – May 2017
2. Maksym Korablyov	M.S. non-thesis	GT Bioinformatics	Feb. 2015 – Aug. 2016

Fulbright Fellow; now working on PhD at MIT Media Lab

1. Mark Wetherington	M.S. non-thesis	GT Physics	Jan. 2014 – Dec. 2014

B3. Undergraduate Students

7. Jinchan Liu	Jilian University, China	Mar. 2019 – current
6. Sarah Bowling	Georgia Tech Physics	Jan. 2019 – current

GT President's Undergraduate Research Award (Fall 2019)

5. Robert Scheiper	Georgia Tech Physics	May 2018 – May 2019
4. Derik Sadowski	Georgia Tech Chemistry	Aug. 2017 – May 2019
3. Evan Seitz	Georgia Tech Physics	Aug. 2016 – May 2017

Started PhD at Columbia Univ. in Fall 2017

2. Alex Covington	Georgia Tech Physics	Nov. 2014 – Aug. 2016

Roger M. Wartell, Ph.D., and Stephen E. Brossette, M.D., Ph.D., Award for Multidisciplinary Studies in Biology, Physics, and Mathematics (Apr. 2016)

H. Fukuyo Outstanding Physics Undergraduate Award (May 2016)
Started MS program in Statistics at Univ. Wisconsin, Madison in Fall 2016

1. Conner Herndon Georgia Tech Physics Jan. 2013 - May 2015
Petit Undergraduate Research Scholar Jan. 2014 – Dec. 2014
Started PhD at Georgia Tech in Fall 2015 in the lab of Flavio Fenton

B4. Service on Thesis Committees (date of defense or proposal given)

Jongwoo Park	Ph.D. student	GT Chem. Eng.	Oct. 2019
Jessica Faubel	Ph.D. student	GT Physics	Aug. 2019
Will Savoie	Ph.D. student	GT Physics	Feb. 2019
Jiyeon Jeong	Ph.D. student	GT Physics	Feb. 2019
Gable Wadsworth	Ph.D. student	GT Physics	Oct. 2018
Shane Jacobeen	Ph.D. student	GT Physics	Oct. 2018
Conner Herndon	Ph.D. student	GT Physics	Oct. 2018
Elaine Rhodes	Ph.D. student	GT Physics	Sept. 2018
Doug Broadwater	Ph.D. student	GT Physics	July 2018
Wenbin Wei	Ph.D. student	GT Physics	May 2018
Asim Alenaizan	Ph.D. student	GT Chemistry	Apr. 2018
Paul Matador	Ph.D. student	GT Bioengineering	July 2017
Dominic Siranni	Ph.D. student	GT Chemistry	Mar. 2017
James Waters	Ph.D. student	GT Physics	Oct. 2016
Patrick Chang	Ph.D. student	GT Physics	Oct. 2016
Tingnan Zhang	Ph.D. student	GT Physics	Mar. 2016
Tung Le	Ph.D. student	GT Physics	Apr. 2015
César Flores	Ph.D. student	GT Physics	July 2014

B5. Mentorship of Postdoctoral Fellows and Visiting Scholars

5. Dr. Atanu Acharya Postdoctoral Associate Jan. 2019 – current
4. Dr. Karl Lundquist Postdoctoral Associate Jan. 2019 – Aug. 2019
3. Ya Wang Graduate student, Dalian University of Technology June 2017 – Sept. 2017
2. Dr. Byeong Chun Postdoctoral Associate Jan. 2016 – Aug. 2016
1. Dr. Anna Pavlova Postdoctoral Associate May 2013 – current

C. Other Teaching Activities

Workshops: All listed are a combination of lectures on molecular dynamics (MD) simulations and hands-on instruction through guided use of written tutorials

July 2018: Dalian, China Biomolecular Dynamics Simulation Workshop 5 days
Lectured 2 days; assisted hands-on for all days

Nov. 2016: Atlanta, GA "Hands-on" Workshop on Computational Biophysics 5 days
Lectured 2 days; led hands-on for all days

June 2015: Melbourne, Australia "Advanced Molecular Modeling Workshop" 3 days
Lectured 1 day; led hands-on 1 day

Jan. 2015: Quintay, Chile "Cryo-EM meets MD Workshop" 4 days
Lectured 1.5 days; led hands-on for all days

Nov. 2014: Atlanta, GA "Hands-on" Workshop on Computational Biophysics 5 days
Lectured 1.5 days; led hands-on for all days

prior to starting at GT

July 2011: Cape Town, South Africa Computational Biophysics workshop 5 days
Lectured 2.5 days; led hands-on for all days

2004-2010: various locations "Hands-on" Workshop on Computational Biophysics 5 days
Assisted hands-on sessions for 12 workshops in total in the US and Europe

VI. Service

A. Professional Contributions

2017-2019: Anton proposal review panel member for the National Academy of Sciences

March 2018: Contributed to the "Data Viz" session at ComSciCon Atlanta, a 2-day workshop for graduate students on science communication.

August 2014: Provided cover image for both first (2008) and second (2014) editions of Membrane Structural Biology by Mary Luckey, Cambridge Press.

Conference Organizing:
Dec. 2013: Organized Atlanta Area Molecular and Cellular Biophysics Symposium

Membership in Professional and Honor Societies:
Biophysical Society

Peer Reviewing:
Manuscripts reviewed (~25 per year) for:
Biophysical Journal, Nature Communications, PLoS Computational Biology, Journal of Membrane Biology, Journal of Chemical Theory and Computation, Journal of Physical Chemistry B, Proceedings of the National Academy of Sciences USA

July 2016: Served as co-editor for a special issue of *Biochimica et Biophysica Acta Biomembranes*, Vol. 1858, Issue 7B

Proposals reviewed for:
NSF, Wellcome Trust (UK), Austrian Science Fund, Lawrence Livermore National Lab, German Research Foundation (DFG)

B. Public and Community Service

Feb. 2019: Judge for Clayton Regional Science and Engineering Fair
Feb. 2018: Judge for Clayton Regional Science and Engineering Fair
Nov. 2017: Judge for Siemens Competition in Math, Science, and Technology (Regional level)
Apr. 2016: PI gave 3D presentations on bacteria and antibiotics to high school students from Gwinnett School of Math, Science, and Technology
Mar. 2016: PI and lab members Gorman Stock and Ben Chun presented VMD Lite at Griffin High School
Dec. 2015: PI and undergraduate Zane Wolf demonstrated the effects of liquid nitrogen at Clayton County Science Day
Mar. 2015: PI and students Karl, Anthony, Conner, and Hyea demonstrated "VMD Lite" to multiple classes at Pope High School in Marietta, GA
Jan. 2015: students Karl, Anthony and Conner participated in Clayton County Science Day
Nov. 2014: Direct-to-discovery (D2D) teleconference with Rabun County Jr. High class
Oct. 2013: Judge for Siemens Competition in Math, Science, and Technology (Regional level)

C. Institute Contributions

Feb. 2019 – Aug. 2019 School of Physics Graduate committee (*interim replacement*)
Sept. 2015 – May 2017 Graduate program committee, Quantitative Biosciences Program (founding member)
Aug. 2015 – Aug. 2017 School of Physics Graduate committee
Sept. 2014 – Mar. 2017 Designed, conducted, and analyzed Physics Alumni survey in which I reached out to ~1,000 graduates of the School of Physics about their education, current occupation, and comments about the program. Results have been and are being used to (1) start an alumni mailing list to increase outreach, (2) design new webpages and advertisements to prospective students, and (3) provide candidates for School of Physics news and events.
Aug. 2013 – Aug. 2015 School of Physics IT committee