

May, 2016

James C. Gumbart, Ph.D.
Assistant 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

Jan. 2013-present Assistant Professor, School of Physics, Georgia Institute of Technology
Dec. 2013-present Adjunct faculty, School of Chemistry & Biochemistry and School of Biology,
Georgia Institute of Technology
Jan. 2011-Jan. 2013 Director's Postdoctoral Fellow, Argonne National Laboratory (advisor: B. Roux)

III. Honors and Awards

2015-2020 NSF CAREER Award
2014 Research featured on the cover of Pittsburgh Supercomputing Center Spring '14 brochure
2011-2013 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 corresponding authorship)

Google Scholar profile at <http://scholar.google.com/citations?user=DOMzcTgAAAAJ&hl=en>

A. Published Books, Parts of Books, and Edited Volumes

A1. Books

No data

A2. Refereed Book Chapters

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, In Press.
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. Other Parts of Books

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

A4. Edited Volumes

No data

B. Refereed Publications and Submitted Articles

B1. Published and Accepted Journal Articles

- 50*. 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.
- 49*. 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*. In press.
- 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.
- Featured in Biophysical Journal's "Best of 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. Gorringer, 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. Strumpf, 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.
Featured in Science Magazine's Editors' Choice: *Science*, 316:1101, 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 (Refereed)

1. Long time and large size molecular dynamics simulations made feasible through new Teragrid hardware and software. Kirby Vandivort, James C. Phillips, Elizabeth Villa, Peter L. Freddolino, **James Gumbart**, Leonardo G. Trabuco, Danielle E. Chandler, Jen Hsin, Christopher B. Harrison, Laxmikant Kale, and Klaus Schulten. *Proceedings of the 2008 TeraGrid Conference*, 2008.

B3. Other Refereed Material

No data

B4. Submitted Journal Articles (with date of submission)

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. Submitted on July 20, 2014.

C. Other Publications (non-refereed)

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

1. Protein:ligand standard binding free energies. Last update Jan. 2014. co-author: C. Chipot
2. Forcing substrates through channels. Last update Sept. 2015 co-author: A. Hazel (graduate student, Physics)
3. Adaptive biasing force calculations in NAMD. Last update Nov. 2014 co-authors: C. Chipot, J. Henin
4. Alchemical free energy perturbation calculations. Last update Nov. 2014 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:

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

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

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

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

16) 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.

15) July 2015: Folding of proteins in distinct environments. Free energy calculations: Three decades of adventure in chemistry and biophysics. Snowmass, CO.

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

- 13) Oct. 2014: A computational glimpse into the peculiar properties of bacterial outer-membrane proteins. Memorial University Biophysics Symposium. St. John's, Newfoundland, Canada.
- 12) July 2014: Exploring the complex free energy landscape of helix formation. Gordon Research Conference on Computational Chemistry. Mount Snow, VT.
- 11) May 2014: Converging on an accurate description of water-membrane partitioning. Workshop on Free Energy Methods in Drug Design. Boston, MA.
- 10) Jan. 2014: Single-molecule views of membrane-protein insertion from MD simulations. XVI Annual Linz Winter Workshop. Linz, Austria.
- 9) Dec. 2013: Outer-membrane protein assembly and insertion. Atlanta-Area Molecular and Cellular Biophysics Symposium. Atlanta, GA.
- 8) July 2013: Membrane-protein insertion at two membranes: Analogous mechanisms at work? Biological membranes and membrane proteins: Challenges for theory and experiment. Snowmass, CO.
- 7) 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.
- 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. James Gumbart, Christophe Chipot, and Klaus Schulten. South African Institute of Physics Conference. Pretoria, South Africa.
- 2) July 2011: Computational microscopy using molecular dynamics. James Gumbart. Biophysics Workshop, South African Institute of Physics Conference. Pretoria, South Africa.
- 1) Sept. 2008: Membrane protein insertion in the translocon. James Gumbart and Klaus Schulten. CECAM Workshop on Membrane Protein Insertion: Theory and Experiment. Lausanne, Switzerland.

Invited presentations at universities & institutes:

- 25) April 2016: Details Matter! Building the Outer Membranes of Gram-Negative Bacteria One Atom at a Time. U. Michigan. Ann Arbor, MI.
- 24) March 2016: Details Matter! Building the Outer Membranes of Gram-Negative Bacteria One Atom at a Time. Clark Atlanta U. Atlanta, GA.
- 23) Nov. 2015: Simulating the periplasmic space of Gram-negative bacteria. RIKEN Institute. Tokyo, Japan.
- 22) Oct. 2015: Simulating the periplasmic space of Gram-negative bacteria. U. Tennessee, Knoxville. Knoxville, TN.
- 21) Sept. 2015: Simulating the periplasmic space of Gram-negative bacteria. Ohio State University. Columbus, OH.
- 20) Jan. 2015: Barreling through the outer membrane one protein at a time. Universidad Andrés Bello. Santiago, Chile.
- 19) Oct. 2014: Barreling through the outer membrane one protein at a time. Oak Ridge National Laboratory. Oak Ridge, TN.

- 18) Aug. 2014: Addressing the arduous problem of calculating free energies of biological processes. Physics Dept. seminar, Chinese University of Hong Kong. Hong Kong, China.
- 17) May 2014: A computational glimpse into the peculiar properties of bacterial outer-membrane proteins. Biochemistry Department Seminar, Emory University. Atlanta, GA.
- 16) Oct. 2013: Assembly and architecture of Gram-positive and –negative cell walls. Biology Department Seminar, Georgia Tech. Atlanta, GA.
- 15) Oct. 2013: Bringing physics to life or: How I learned to stop worrying and love biology. Society of Physics Students, Georgia Tech. Atlanta, GA.
- 14) Aug. 2013: Mechanisms of membrane-protein insertion at the inner and outer membranes. Molecular Biophysics Research Review, Georgia Tech. Atlanta, GA.
- 13) 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.
- 12) April 2013: Mechanisms of SecM-mediated stalling in the ribosome. RiboEvo Seminar, Georgia Tech. Atlanta, GA.
- 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.

Contributed presentations at conferences:

- 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. James Gumbart. 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. James Gumbart, Christophe Chipot, and Klaus Schulten. Biophysical Society Annual Meeting. San Francisco, CA.

2) Feb. 2009: Regulation of the protein-conducting channel by a bound ribosome. James Gumbart, Leonardo G. Trabuco, Elizabeth Villa, Eduard Schreiner, Christopher B. Harrison, Klaus Schulten. Biophysical Society Annual Meeting. Boston, MA.

1) Feb. 2007: Mechanics of force propagation in TonB-dependent outer membrane transporters. James Gumbart, Michael C. Wiener, and Emad Tajkhorshid. Biophysical Society Annual Meeting. Baltimore, MD.

E. Grants and Contracts

E1. As Principal Investigator

Research Grants and Contracts:

Currently funded:

06/01/2015 – 05/31/2020 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

05/15/2013 – 05/14/2016 NIH K22-AI100927 \$268,585 total (\$250,000 direct) PI
Combating infection through atomic-scale modeling of unique bacterial systems
Currently on a 1-year no-cost extension.

05/15/2014 – 12/31/2015 BWF Travel Award \$9,950 total PI
Development of novel approaches and models for permeability calculations

10/01/2015 – 09/30/2016 NSF XRAC MCB130173 15.48 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 \$575,891.58 according to NSF.

11/01/2014 – 10/31/2015 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.

Previous funding:

10/01/2014 – 09/30/2015 NSF XRAC MCB130173 6.92 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

11/01/2013 – 10/31/2014 Anton PSCA13032P 100,000 CPU-hours PI
Determining the mechanisms of protein folding in membranes

10/01/2013 – 09/30/2014 NSF XRAC MCB130173 6.5 million CPU-hours PI
Structure and dynamics of bacteria-specific systems

11/01/2012 – 10/31/2013 Anton PSCA12028P 100,000 CPU-hours PI
Determining the mechanisms of protein folding in membranes

E2. As Co-Principal Investigator

Currently funded:

04/01/2013 – 03/31/2018 NIH R01-GM101425 \$113,000 direct to JCG Co-I
Structural basis of chemoreception. PI: Grant Jensen (Caltech)

07/01/2015 – 06/30/2016 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)

Previous funding:

07/01/2013 – 06/30/2015 NIH R01-GM067887 \$123,000 direct to JCG Co-I
Mechanisms of membrane proteins through in-situ modeling. PI: Klaus Schulten (UIUC)

E3. As Senior Personnel or Contributor

No data

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) remains one of the top 20 most accessed in Journal of Computational Chemistry.

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.

G. Societal and Policy Impacts

No data

H. Other Professional Activities

No data

V. Teaching

A. Courses Taught

| | | | |
|-------------|--------------|------------------|--------------|
| Spring 2016 | Physics 4251 | Biophysics | 14 students |
| Fall 2015 | Physics 4601 | Senior Seminar I | 24 students |
| Fall 2015 | Physics 2211 | Intro Physics I | 170 students |
| Fall 2014 | Physics 4251 | Biophysics | 11 students |
| Fall 2013 | Physics 4251 | Biophysics | 10 students |

B. Individual Student Guidance

B1. PhD Students

| | | |
|-------------------|---|----------------------|
| 5. Hennem Hwang | GT Materials Science & Engineering | Dec. 2014 - current |
| 4. Gorman Stock | GT Chemistry | Jan. 2014 - current |
| 3. Karl Lundquist | GT Physics | Jan. 2014 - current |
| | GAANN fellowship recipient Aug. 2013 – Aug. 2015 | |
| 2. Anthony Hazel | GT Physics | April 2013 - current |
| 1. Curtis Balusek | GT Physics | Jan. 2013 – current |
| | GAANN fellowship recipient Aug. 2013 – Aug. 2015 | |
| | Bonnie B. and Charles K Rice Jr. Fellowship Aug. 2015 – Aug. 2016 | |

B2. M.S. students

| | | | |
|----------------------|-----------------|-------------------|---------------------|
| 2. Maksym Korablyov | M.S. non-thesis | GT Bioinformatics | graduated Dec. 2015 |
| 1. Mark Wetherington | M.S. non-thesis | GT Physics | graduated Dec. 2014 |

B3. Undergraduate Students

| | | |
|-------------------|----------------------------|---------------------|
| 2. Alex Covington | Georgia Tech Physics major | Nov. 2014 – current |
|-------------------|----------------------------|---------------------|

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

1. Conner Herndon Georgia Tech Physics major Jan. 2013 - May 2015
Petit Undergraduate Research Scholar Jan. 2014 – Dec. 2014

B4. Service on Thesis Committees

| | | | |
|---------------|---------------|----------------------|---------------|
| Jiyeon Jeong | Ph.D. student | Georgia Tech Physics | April 2016 |
| Tingnan Zhang | Ph.D. student | Georgia Tech Physics | March 2016 |
| Patrick Chang | Ph.D. student | Georgia Tech Physics | February 2016 |
| Wenbin Wei | Ph.D. student | Georgia Tech Physics | January 2016 |
| Tung Le | Ph.D. student | Georgia Tech Physics | April 2015 |
| César Flores | Ph.D. student | Georgia Tech Physics | July 2014 |

B5. Mentorship of Postdoctoral Fellows and Visiting Scholars

2. Dr. Byeong Chun Postdoctoral Fellow Jan. 2016 – current
1. Dr. Anna Pavlova Postdoctoral Fellow May 2013 – current

C. Other Teaching Activities

Fall 2015: Updated Physics 4601, Senior Seminar, which originally only required attending GT Physics faculty presentations once per week, to now focus on GRE subject test preparation, graduate school applications, and careers outside of academia.

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

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

Conference Organizing:

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

Membership in Professional and Honor Societies:

Biophysical Society

Peer Reviewing:

Manuscripts reviewed (~15 per year total) 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

Proposals reviewed for:

NSF, Austrian Science Fund, Lawrence Livermore National Lab

B. Public and Community Service

April 2016: PI gave 3D presentations on bacteria and antibiotics to high school students from Gwinnett School of Math, Science, and Technology

March 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

March 2015: PI and students Karl, Anthony, Conner, and Hennim 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

Sept. 2015 – current Graduate program committee, Quantitative Biosciences Program (founding member)

Aug. 2013 – Aug. 2015 School of Physics IT committee

Aug. 2015 – current School of Physics Graduate committee

Aug. 2015 – current School of Physics communications committee (founding member)