

## Curriculum Vitae and Table of Contents

James C. Gumbart, Ph.D.

Associate Professor

School of Physics

Georgia Institute of Technology

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September 2021

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### **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 Biosciences, Georgia Institute of Technology  
2020-present Associate Director, Quantitative Biosciences Graduate Program

### **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  
2013 NIAID K22 Career Transition Award  
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 when not last author)

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

Scopus profile at <https://www.scopus.com/authid/detail.uri?authorId=8553717000>

### **A. Published Books, Book Chapters, and Edited Volumes**

#### **A1. Books**

No data

#### **A2. Refereed Book Chapters**

6. **Li Y@, Liu J@, Gumbart JC.** Preparing membrane proteins for simulation using CHARMM-GUI. In *Structure and Function of Membrane Proteins*, I. Schmidt-Krey and J. C. Gumbart, Eds. Springer, 237-251, 2021.
5. **Balusek C, Hwang H, Hazel A, Lundquist K, Pavlova A, Gumbart JC.** Diverse Protein-Folding Pathways and Functions of  $\beta$ -Hairpins and  $\beta$ -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

*Google Scholar h-index: 38; 31 since 2016*

#### B1. Published and Accepted Journal Articles

104\*. Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. **J.C. Gumbart\***, J.L. Ferreira, **H. Hwang**, **A.J. Hazel**, C. Cooper, J.M. Parks, J.C. Smith, H.I. Zgurskaya, and M. Beeby. *Biophysical Journal*. In press.

103\*. Quantifying Arrhythmic Long-QT Effects of Hydroxychloroquine and Azithromycin with Whole Heart Optical Mapping and Simulations. I. Uzelac\*, A. Kaboudian\*, S. Irvanian, J.G. Siles-Paredes, **J. C. Gumbart**, H. Ashikaga, N. Bhatia, R. F. Gilmour Jr., E. M. Cherry, and F. H. Fenton. *Heart Rhythm O2*. In press.

102\*. Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. **A. Pavlova**, **Z. Zhang**, **A. Acharya**, **D.L. Lynch**, **Y.T. Pang**, Z. Mou, J.M. Parks, C. Chipot\*, and **J.C. Gumbart\***. *J. Physical Chemistry Letters*. 12:5494-5502, 2021.

101\*. Combinatorial phosphorylation modulates the structure and function of the G protein gamma subunit in yeast. Z.N. Toosi, X. Su, R. Austin, S. Choudhury, W. Li, **Y.T. Pang**, **J.C. Gumbart**, and M. P. Torres. *Science Signaling*. 14:eabd2464, 2021.

100\*. Inward-facing glycine residues create sharp turns in  $\beta$ -barrel membrane proteins. **Z. Zhang**, **D. Ryoo**, **C. Balusek**, **A. Acharya**, M. Orwick Rydmark, D. Linke, and **J.C. Gumbart**. *Biochimica et Biophysica Acta (BBA) – Biomembranes*. 1863:183662, 2021.

99\*. ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV. **A. Acharya\***, **D.L. Lynch**, **A. Pavlova**, **Y.T. Pang**, and **J.C. Gumbart\***. *Chemical Communications*. 57:5949-5952, 2021.

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97\*. Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. L. Zanetti-Polzi, M.D. Smith, C. Chipot, **J.C. Gumbart**, **D.L. Lynch**, **A. Pavlova**, J.C. Smith, and I. Daidone. *J. Physical Chemistry Letters*. 12:4195-4202, 2021.

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- 94\*. Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. **A. Pavlova**, **D.L. Lynch**, I. Daidone, L. Zanetti-Polzi, M.D. Smith, C. Chipot, D.W. Kneller, A. Kovalevsky, L. Coates, A.A. Golosov, C.J. Dickson, C. Velez-Vega, J.S. Duca, J. V. Vermaas, **Y.T. Pang**, **A. Acharya**, J.M. Parks, J.C. Smith, and **J.C. Gumbart**. *Chemical Science*. 12: 1513-1527, 2021.
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- 91\*. A Novel Approach to Simulating the Gating Transitions of Mechanosensitive Channels. **J.C. Gumbart**. *Biophysical Journal*. 120:185-186, 2021.
- 90\*.  $\beta$ -Barrel Proteins Tether the Outer Membrane in Many Gram-Negative Bacteria. K. M. Sandoz, R.A. Moore, P.A. Beare, A. V. Patel, R. E. Smith, M. Bern, **H. Hwang**, C. J. Cooper, S. A. Priola, J.M. Parks, **J.C. Gumbart**, S. Mesnage, and R. A. Heinzen. *Nature Microbiology*. 6:19-26, 2021.
- 89\*. Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. **A. Acharya**, R. Agarwal, M. Baker, J. Baudry, D. Bhowmik, S. Boehm, K. Byler, L. Coates, S.Y.-C. Chen, C.J. Cooper, O. Demerdash, I. Daidone, J. Eblen, S.R. Ellingson, S. Forli, J. Glaser, **J.C. Gumbart**, J. Gunnels, O. Hernandez, S. Irle, J. Larkin, T.J. Lawrence, S. LeGrand, S.-H. Liu, J.C. Mitchell, G. Park, J.M. Parks, **A. Pavlova**, L. Petridis, D. Poole, L. Pouchard, A. Ramanathan, D. Rogers, D. Santos-Martins, A. Scheinberg, A. Sedova, S. Shen, J.C. Smith, M.D. Smith, C. Soto, A. Tsaris, M. Thavappiragasam, A.F. Tillack, J.V. Vermaas, V. Q. Vuong, J. Yin, S. Yoo, M. Zahran, L. Zanetti-Polzi. *J. Chemical Information and Modeling*. 60:5832–5852, 2020.
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- 81\*. Outer membrane protein size and LPS O-antigen define protective antibody targeting to the *Salmonella* surface. C.C. Domínguez-Medina, M. Pérez-Toledo, A.E. Schager, J.L. Marshall, C.N. Cook, S. Bobat, **H. Hwang**, **B.J. Chun**, E. Logan, J.A. Bryant, W.M. Channell, F.C. Morris, S. Jossi, A. Alshayea, A.E. Rossiter, P.A. Barrow, W.G. Horsnell, C.A. MacLennan, I.R. Henderson, J. Lakey, **J.C. Gumbart**, C. López-Macías, V.N. Bavro, and A.F. Cunningham. *Nature Communications*. 11:851, 2020.
- 80\*. A minimal membrane metal transport system: Dynamics and energetics of *mer* proteins. **H. Hwang**, **A. Hazel**, P. Lian, J.C. Smith, **J.C. Gumbart\***, and J.M. Parks\*. *J. Computational Chemistry*. 41:528-537, 2020.
- 79\*. Presence of substrate aids lateral gate separation in LptD. **K.P. Lundquist** and **J.C. Gumbart\***. *Biochimica et Biophysica Acta (BBA) – Biomembranes*. 1862:183025, 2020.
- 78\*. Non-detergent isolation of a cyanobacterial photosystem I using styrene maleic acid alternating copolymers. N.G. Brady, M. Li, Y. Ma, **J.C. Gumbart**, and B.D. Bruce. *RSC Advances*. 9:31781-31796, 2019.
- 77\*. 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*. 5:1926-1935, 2019.
- 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. *Chemical Communications*. 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  $\beta$  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  $\beta$ -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<sup>1</sup>, **K. Lundquist<sup>1</sup>, H. Hwang<sup>1</sup>**, 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. <sup>1</sup>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  $\beta$ -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.
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- 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.
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- 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.
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**Lundquist, C. Herndon@**, T.H. Harty, and **J.C. Gumbart**. *Biochemistry and Molecular Biology Education*. 44:124-129, 2016.

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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.

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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.



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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<sup>+</sup> 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. *Biophysical Journal*, 103:331-341, 2012.
23. Determination of membrane-insertion free energies by molecular dynamics simulations. **J. Gumbart** and B. Roux. *Biophysical Journal*, 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. Goringe, 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. *Biochimica et Biophysica Acta (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. *Biophysical Journal*, 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. *Biophysical Journal*, 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. *Biophysical Journal*, 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. *Biophysical Journal*, 93:496-504, 2007.
3. Molecular dynamics studies of the archaeal translocon. **J. Gumbart** and K. Schulten. *Biophysical Journal*, 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. Membrane Protein Tutorial Last update Dec. 2020 co-authors: Yupeng Li, Jinchan Liu (undergraduate students)
2. Protein:ligand standard binding free energies. Last update Sept. 2017 co-author: C. Chipot
3. Forcing substrates through channels. Last update Sept. 2017 co-author: A. Hazel (graduate student, Physics)
5. Adaptive biasing force calculations in NAMD. Last update Sept. 2017 co-authors: C. Chipot, J. Henin
5. 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:

- 31) August 2021: Opening of BamA's lateral gate is regulated by other members in the BAM complex. American Chemical Society National Meeting. Atlanta, GA.
- 30) Critical interactions for SARS-CoV-2 spike protein binding to ACE2 identified by machine learning. August 2021: American Chemical Society National Meeting. Atlanta, GA.
- 29) April 2021: Free-energy calculations of SARS-CoV-2 spike protein opening. American Chemical Society National Meeting. Virtual meeting.
- 28) March 2021: Automated identification of critical interactions for coronavirus S protein binding to ACE2. Georgia Tech Hive Symposium, Georgia Tech, Atlanta GA.
- 27) March 2021: Modeling the Bacterial Cell Envelope at Atomistic Resolution. Bacterial Cell Envelopes, Structure, Dynamics, Function. University of Southampton Virtual Symposium.
- 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.

***Invited presentations at universities & institutes:***

- 30) August 2021: Using petascale supercomputing to quantify the S-protein closed-to-open transition. Workshop on Big data and machine learning against COVID-19. Universidad de Ingenieria y Tecnologia (UTEC), Lima, Peru.
- 29) August 2021: Dissecting coronavirus binding with atomistic molecular dynamics simulations and machine learning. Workshop on Big data and machine learning against COVID-19. Universidad de Ingenieria y Tecnologia (UTEC), Lima, Peru.
- 28) February 2021: MD simulations, free-energy calculations, and machine learning applied to SARS-CoV-2 proteins. Society of Physics Students, Georgia Tech, Atlanta, GA.
- 27) January 2021: MD simulations, free-energy calculations, and machine learning applied to SARS-CoV-2 proteins. Colorado School of Mines, Golden, CO.
- 26) November 2020: MD simulations, free-energy calculations, and machine learning applied to SARS-CoV-2 proteins. University of Illinois, Urbana-Champaign, Urbana, IL.
- 25) October 2019: Protein folding at the Gram-negative outer membrane. National Institutes of Health, Bethesda, MD.

- 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  $\beta$ -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.

***Contributed presentations at conferences:***

- 6) Feb. 2020: Targeting multidrug efflux with large-scale atomistic simulations. Biophysical Society Annual Meeting. San Diego, CA.
- 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:

06/2020 – 05/2025	NIH R01-AI148740	\$1,979,750 (\$1,250,000 direct)	PI
	Altering Hepatitis B Virus assembly through pharmacological intervention		
09/2017 – 06/2022	NIH R01-GM123169	\$1,400,398 (\$1,011,687 direct)	PI
	Dynamic characterization of outer-membrane-protein biogenesis by the BAM and TAM complexes		
08/2020 – 12/2021	Bristol Myers Squibb	\$74,624 (\$53,047 direct)	PI
	Extending the Force-field Toolkit in VMD to support the Psi4 QM package		

Previous funding:

01/2021 – 06/2021	GT Research Institute	\$110,655	PI
	BioVLSI – Very Large Scale Integration		
06/2015 – 05/2021	NSF MCB-1452464	\$797,773 (\$586,200 direct)	PI
	CAREER: Research and education on protein folding as an energy source at the bacterial outer membrane		
05/2013 – 05/2016	NIH K22-AI100927	\$268,585 (\$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		

Supercomputer time

03/2021 – 03/2022	NSF XRAC MCB130173	5.43 million CPU-hours	PI
	Structure and dynamics of bacteria-specific systems		
05/2020 – 10/2020	COVID-19 HPC Consortium	95,000 Summit node-hours	PI



Determining the contribution of glycosylation to SARS-CoV-2 S-protein conformational dynamics

*We received a sizeable allocation on the US's fastest supercomputer, Summit, to carry out COVID-related simulations.*

10/2019 – 03/2021	NSF XRAC MCB130173	10.37 million CPU-hours	PI
	Structure and dynamics of bacteria-specific systems		
10/2018 – 09/2019	NSF XRAC MCB130173	9.72 million CPU-hours	PI
	Structure and dynamics of bacteria-specific systems		
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)		
	<i>DOE's INCITE program provides computational time on the fastest supercomputers in the nation. This project was one of only four selected in the field of biophysics.</i>		
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		
11/2014 – 10/2015	Anton PSCA14044P	100,000 CPU-hours	PI
	Determining the mechanisms of protein folding in membranes		
	<i>Anton is a special-purpose supercomputer developed by DE Shaw Research.</i>		
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:

08/2021 – 06/2022	GT Research Institute	\$125,000	Co-PI
	SyMBioTE: <u>S</u> ystemic <u>M</u> odeling for <u>B</u> iological <u>T</u> ransistor <u>E</u> valuation.		
09/2020 – 08/2023	NSF CLP 2004030	\$34,270 (\$21,663 direct to JCG)	Co-PI
	Collaborative Research: Constructing and employing pyrroles in natural product biosynthetic pathways. PI: Vinayak Agarwal (Georgia Tech)		
09/2018 – 08/2023	NSF PHY-1806833	\$1,909,529 total	Co-PI
	Collaborative Research: Formation of a High Flux Student Research Network		

## **E3. As Senior Personnel or Contributor**

Currently funded: *Numbers represent GT's portion*

04/2021 – 03/2023	NIH R21-AI160107	\$106,786 (\$67,500 direct)	Co-I
	Defining the molecular mechanisms of COPA syndrome through computational modeling and functional studies. PI: Anthony Shum (UCSF)		
04/2020 – 03/2025	NIH R01-AI116525	\$148,932 (\$94,381)	Co-I

MmpL3 as a target for novel anti-TB agents. PI: Mary Jackson (Colorado St.)

06/2020 – 05/2025 NIH R01-AI052293 \$331,835 (\$235,105) Co-I  
Transport across two membranes by AcrAB-TolC. PI: Helen Zgurskaya (Oklahoma St.)

Previous funding:

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

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

## 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 almost 400 citations.

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 2021	Physics 4251/6250	Biophysics	14 students
Spring 2021	Physics 8901GM	QBioS Workshop	8 students
Spring 2021	Physics 4601	Senior Seminar I	59 students
Fall 2020	Physics 4251/6250	Biophysics	26 students
Spring 2020	Physics 4601	Senior Seminar I	46 students
Spring 2020	Physics 2212	Intro Physics of Living Systems II	75 students
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

- |                   |                                                                                                  |                         |
|-------------------|--------------------------------------------------------------------------------------------------|-------------------------|
| 10. Zixing Fan    | GT Bioengineering                                                                                | Aug. 2021 – current     |
| 9. Yunlin Zeng    | GT Physics                                                                                       | Feb. 2021 – current     |
| 8. Katie Kuo      | GT Chemistry                                                                                     | Oct. 2018 – current     |
|                   | First Place Talk, School of Chemistry and Biochemistry Graduate Research Symposium (Spring 2021) |                         |
| 7. Zijian Zhang   | GT Physics                                                                                       | Dec. 2017 – current     |
|                   | GT-ORNL Seed Grant recipient Jan. 2021                                                           |                         |
| 6. David Ryoo     | GT Bioengineering                                                                                | Oct. 2017 – current     |
| 5. Yui Tik Pang   | GT Physics                                                                                       | Aug. 2017 – current     |
|                   | Frontera Computational Science Fellowship July 2021 – June 2022                                  |                         |
| 4. Hyea Hwang     | GT Materials Science & Eng.                                                                      | Dec. 2014 – Jan. 2019   |
|                   |                                                                                                  | <i>Defended 12/2018</i> |
|                   | DOE SCSGR Award recipient to work at Oak Ridge National Lab (11/2017-7/2018)                     |                         |
| 3. Karl Lundquist | GT Physics                                                                                       | Jan. 2014 – Jan. 2019   |
|                   |                                                                                                  | <i>Defended 12/2018</i> |
|                   | GAANN fellowship recipient Aug. 2013 – Aug. 2015                                                 |                         |
| 2. Anthony Hazel  | GT Physics                                                                                       | Apr. 2013 – Jan. 2019   |
|                   |                                                                                                  | <i>Defended 12/2018</i> |
|                   | Larry S. O'Hara Fellowship Jan. 2017 – Dec. 2017                                                 |                         |
| 1. Curtis Balusek | GT Physics                                                                                       | Jan. 2013 – Jan. 2019   |
|                   |                                                                                                  | <i>Defended 12/2018</i> |
|                   | 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; went on to PhD at MIT Media Lab |                       |
| 1. Mark Wetherington | M.S. non-thesis GT Physics                        | Jan. 2014 – Dec. 2014 |

### B3. Undergraduate Students

- |                    |                                                           |                        |
|--------------------|-----------------------------------------------------------|------------------------|
| 12. Jiyun Zhang    | Smith College                                             | May 2021 – July 2021   |
|                    | Chemistry REU student                                     |                        |
| 11. Shauna Wallock | Georgia Gwinnett College                                  | May 2021 – July 2021   |
|                    | Chemistry REU student                                     |                        |
| 10. Yang Lixinhao  | Jilin University, China                                   | July 2020 – current    |
| 9. Morgan Brinson  | American University                                       | May 2020 – August 2020 |
|                    | Started PhD at Rice Univ. in Fall 2021                    |                        |
| 8. Yupeng Li       | Jilin University, China                                   | Dec. 2019 – Aug. 2021  |
|                    | Started PhD at U. Illinois, Urbana-Champaign in Fall 2021 |                        |
| 7. Jinchan Liu     | Jilin University, China                                   | Mar. 2019 – Aug. 2020  |
|                    | Started PhD at Yale Univ. in Fall 2020                    |                        |
| 6. Sarah Bowling   | Georgia Tech Physics                                      | Jan. 2019 – Dec. 2020  |
|                    | 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)

Conner Herndon	Ph.D. student	GT Physics	Jul. 2021
Alicia Robang	Ph.D. student	GT Chem. Eng.	Jun. 2021
Emily Saccuzzo	Ph.D. student	GT Chemistry	Jun. 2021
Ziying Cao	Ph.D. student	GT Chemistry	April 2021
Jessica Faubel	Ph.D. student	GT Physics	April 2021
Asim Alenaizan	Ph.D. student	GT Chemistry	Mar. 2021
Alec Cook	Ph.D. student	GT Physics	Dec. 2020
Siyang Cen	Ph.D. student	GT Chemistry	April 2020
Dongqi Yi	Ph.D. student	GT Chemistry	April 2020
Suehyun Park	Ph.D. student	GT Chemistry	April 2020
Dominic Siranni	Ph.D. student	GT Chemistry	Mar. 2020
David Yanni	Ph.D. student	GT Physics	Nov. 2019
Jongwoo Park	Ph.D. student	GT Chem. Eng.	Oct. 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
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
Paul Matador	Ph.D. student	GT Bioengineering	July 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**

6. Dr. Diane Lynch      Research Scientist      May 2020 – current
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  
Research Scientist I since May 2018

### **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**

Jan. 2020: NSF reviewer

2017-2021: Anton proposal review panel member for the National Academy of Sciences  
**2021**: Chair of NAS Review Committee

2019-2020: XSEDE User Requirements Evaluation and Prioritization team

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:***

April 2021: Co-organized “A Call to Action: The Many Roles of Computational Chemistry in Addressing COVID-19” symposium for American Chemical Society meeting

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

#### ***Membership in Professional and Honor Societies:***

Biophysical Society, American Chemical Society

#### ***Peer Reviewing:***

Manuscripts reviewed (~30 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), French National Agency for Research (ANR)

**B. Public and Community Service**

Feb. 2021: Judge for Clayton Regional Science and Engineering Fair (virtual)  
Oct. 2020: Supercomputing 2020 Virtual Career Panel  
Feb. 2020: Judge for Clayton Regional Science and Engineering Fair  
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**

Aug. 2021 – current School of Physics Strategic Planning Committee  
April 2021 Reviewer, Institute TA awards  
March 2021 – current GT College of Sciences Academic Faculty Advisory Council  
August 2020 – current Physics Undergraduate Research Task Force  
August 2020 – current Associate Director of Quantitative Biosciences Graduate Program  
-Developed and organized alumni career seminar series each semester  
-Assisted design and implementation of virtual recruitment event  
-Led first-year cohorts in designing, advertising, and carrying out Spring modeling workshops  
July 2020 – Aug. 2021 School of Physics Diversity, Equity, and Inclusion Task Force  
Feb. 2019 – Aug. 2019 School of Physics Graduate committee (*interim replacement*)  
Sept. 2015 – May 2017 Graduate program committee, Quantitative Biosciences Graduate 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