Troy A. Brier

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Professional Summary

Computational chemist with a background in biological scientific computing. Experienced solving diverse problems in computational science settings applying novel techniques across domains. Skilled in the design and management of exploratory multi-year projects requiring flexibility, self-assessment mechanisms, and documentation suitable for publication. Proficient in presenting technical material to audiences with varying subject-matter expertise.

Education

University of Illinois at Urbana-Champaign (UIUC)	**PhD in Chemistry**	*Aug 2017 – Dec 2024*
The College of New Jersey (TCNJ)	**BS in Chemistry (ACS-certified)**	*Aug 2013 – May 2017*

Awards

Young Scholars Outstanding Mentor Awardee	UIUC	*Summer 2018*
Alfred P. Sloan Fellow	UIUC	*Fall 2017*
Rodger Adams Fellow	UIUC	*Fall 2017*
Hannum Fellow	UIUC	*Fall 2017*
Goodkin Physical Chemistry Awardee	TCNJ	*Spring 2017*
Research Experience for Undergraduate (REU)	Colorado State University	*Summer 2016*
Mentored Undergraduate Summer Experience (MUSE)	TCNJ	*Summer 2015*
TCNJ Chairman of the Board Scholar	TCNJ	*All Semesters*

Research Experience

Graduate/Postdoctoral Research Assistant | *The Luthey-Schulten Group*, Dept. of Chemistry at UIUC *Jan 2018 – present*

- Doctoral Dissertation: Shaping the bacterial transcriptome: Perspectives from kinetic modeling
- Constructed a stochastic kinetic model using data collected from super-resolution imaging experiments to simulate the sugar-stress response in *Escherichia coli*.
- Collaborated in the use of GPU-accelerated, hybrid stochastic-deterministic methods to simulate whole-cell models of bacteria that capture the reaction and diffusion of ∼10,000 biochemical components at the cell-scale.
  * Constructed a kinetic model of the nucleotide metabolism for a bacteria cell.
  * Curated genomics, transcriptomics, proteomics, metabolomics, and kinetic rates data.
  * Updated software/code for use on high performance GPU cluster.
- Developed a methodology to profile the bacterial transcriptome coupling bioinformatics and experiment.
  * Built a sequence alignment based pipeline to identify genetic motifs within a bacterial genome and predict transcriptional events.
  * Analyzed Illumina, Pacific Biosciences, and Oxford Nanopore Technologies RNA sequencing experiments.
  * Created tools to predict transcription units and visualize the RNA isoforms.
- Assisted PI in preparation of grant materials to acquire federal funding: *NSF MCB 2221237* - $2.00M (proposal, annual reports) | *NSF MCB 1818344* - $1.50M (annual reports) | *NSF MCB 1840320* - $1.18M (annual reports).
- Maintained group's GPU cluster and website.
- Collaborated with industrial and academic partners, both domestic and international.
- Presented research results to broader scientific community at domestic and international conferences.
- Mentored junior graduate and undergraduate student researchers.

Undergraduate Research Assistant | *The Baker Group*, Dept. of Chemistry at TCNJ *Dec 2014 – May 2017*

- Explored individual and multiplte type IV bacterial pilin subunit(s) dynamics and aggregation in a membrane environment using atomistic and MARTINI coarse grained molecular dynamics simulations.
- Presented research results to broader scientific community at domestic conferences.
- Mentored junior undergraduate student researchers.

REU Summer Research Intern | *The McCullagh Group*, Dept. of Chemistry at Colorado State University *May 2016 – July 2016*

- Worked in the McCullagh Group for a ten-week program consisting of a two week computational chemistry course and a eight week research period.
- Performed molecular dynamics simulations to develop methodology for ligand binding site identification to aid drug design.
- Presented poster of results at a poster session.

MUSE Research Intern | *The Baker Group*, Dept. of Chemistry at TCNJ *Summer 2015*

- Worked in the Baker Biomoleculer Modeling and Simulation group for an eight week program
- Investigated the effect membrane environments have on type IV pilin subunits from *Neisseria gonorrhoeae* and *Pseudomonas aeruginosa* using atomistic molecular dynamics simulations.
- Presented research results to broader scientific community at poster session.

Teaching Experience

STC-QCB Advance Computational Workshop Teaching Assistant | NSF STC-QCB at UIUC *May 2024*
- Served as a mentor to teaching assistants helping to construct and test tutorials to teach about stochastic whole-cell modeling.
- Installed software used during the workshop to run simulations on supercomputer.
- Performed minor task as a teaching assistant helping to troubleshoot during the workshop.

Workshop Teaching Assistant | NIH Resource for Macromolecular Modeling and Bioinformatics at UIUC *October 2021*
- Served as a teaching assistant for the online hands-on workshop on computational biophysics hosted by the NIH Resource for Macromolecular Modeling and Bioinformatics.
- Instructed graduate students and post-doctoral associates from different schools on simulation techniques using the Lattice Microbes stochastic simulation package.

Statistical Thermodynamics Teaching Assistant | Dept. of Chemistry at UIUC *Fall 2019*
- Prepared course materials, graded, and hosted office hours.

Instrumental Analysis Teaching Assistant | Dept. of Chemistry at UIUC *Fall 2017, Fall 2019*
- Supervised laboratory sessions for multiple instruments, prepared course materials, graded, and hosted office hours.

CPLC Summer School Teaching Assistant | NSF CPLC at UIUC *July 2019*
- Served as a teaching assistant for summer school hosted by the NSF Center for the Physics of Living Cells (CPLC) Summer School—Held lectures for graduate students and post-doctoral associates and prepared tutorials run on AWS instances.
- Graduate students and post-doctoral associates from different schools visit the UIUC to learn new techniques. With fellow collaborators, instructed the students on how to perform super resolution imaging experiments and combine the data with computational techniques.

Math and Science Tutor | Tutoring Center at TCNJ *Fall 2019 - Spring 2017*
- Tutored fellow students in Calculus I, General Chemistry I, General Chemistry II, Physics 201, Computer Programming I (Java) through the tutoring center. My objective was to provide students with the tools necessary to succeed in their respective courses.

Publications (0000-0002-9530-6517)

T. A. Brier, J. E. Cournoyer, B. R. Gilbert, S. A. Glass, Y. Gao, Z. R. Thornburg, K. Goglin, G. John, T. Mamaghani, S. Shivakumar, Y. Yu, C. Fields, J. I. Glass, A. P. Mehta, Z. Luthey-Schulten, **Unraveling the Transcriptional Landscape within a Minimized Bacterium via Comparative Analysis**, *in preparation*

T. E. Long, Z. R. Thornburg, B. R. Gilbert, T. A. Brier, Z. Luthey-Schulten, J. I. Glass (ed.), **Chapter — Determining the Rules of Life of the Minimal Cell Using Whole-Cell Simulation**, *Minimal Genomes and Their Applications, Royal Society of Chemistry 2024, (in press)*

B. R. Gilbert, Z. R. Thornburg, T. A. Brier, J. A. Stevens, F. Grünewald, J. E. Stone, S. J. Marrink, Z. Luthey-Schulten, **Dynamics of Chromosome Organization in a Minimal Bacterial Cell**, *Frontiers in Cell and Developmental Biology 2023*

J. A. Stevens, F. Grünewald, P.A. Marco van Tilburg, M. König, B. R. Gilbert, T. A. Brier, Z. R. Thornburg, Z. Luthey-Schulten, S. J. Marrink, **Molecular Dynamics Simulation of an Entire Cell**, *Frontiers in Chemistry 2023*

Z. R. Thornburg, D. M. Bianchi, T. A. Brier, B. R. Gilbert, T. M. Earnest, M. C.R. Melo, N. Safronova, J. P. Sáenz, A. T. Cook, K. S. Wise, C. A. Hutchison III, H. O. Smith, J. I. Glass, Z. Luthey-Schulten, **Fundamental Behaviors Emerge from Simulations of a Living Minimal Cell**, *Cell 2022*

D. M. Bianchi, T. A. Brier, A. Poddar, M. S. Azam, C. K. Vanderpool, T. Ha, Z. Luthey-Schulten, **Stochastic Analysis Demonstrates the Dual Role of Hfq in Chaperoning *E. coli* Sugar Shock**, *Frontiers in Molecular Biosciences 2020*

Z. R. Thornburg, M. C.R. Melo, D. M. Bianchi, T. A. Brier, C. Crotty, M. Breuer, H. O. Smith, C. A. Hutchison III, J. I. Glass, Z. Luthey-Schulten, **Kinetic Modeling of the Genetic Information Processes in a Minimal Cell**, *Frontiers in Molecular Biosciences 2019*

Presentations (0000-0002-9530-6517)

Impact of gene expression strategies in near whole-cell models of minimal bacteria *Biophysical Society Meeting 2024*
- T. A. Brier, J.E. Cournoyer, B.R. Gilbert, Z.R. Thornburg, J.I. Glass, C.J. Fields, A.P. Mehta, and Z. Luthey-Schulten
- *Seminar* presented at the annual Biophysical Society Meeting Feb. 2024 in Philadelphia, PA

Stochastic simulations of varied gene expression models within minimal bacteria *JCVI Minimal Workshop 2023*
- T. A. Brier, B.R. Gilbert, J.I. Glass, and Z. Luthey-Schulten
- *Seminar* presented virtually for the JCVI Minimal Workshop 2023, Sept. 2023

Towards deciphering the influence of genome architecture in minimized bacteria *Sloan UCEM Conference 2023*
- T. A. Brier, P. Venepally, J.I. Glass, and Z. Luthey-Schulten
- *Seminar* presented at the 8th Annual Sloan UCEM Conference, Apr. 2023 in Urbana, IL

Deciphering the influence of genome architecture in minimized bacteria *Biophysical Society Meeting 2023*
- T. A. Brier, P. Venepally, J.I. Glass, and Z. Luthey-Schulten
- *Poster* presented at the annual Biophysical Society Meeting Feb. 2023 in San Deigo, CA.

Deciphering the influence of genome architecture in JCVI-syn1.0 *JCVI Minimal Workshop 2022*
- T. A. Brier, J.I. Glass, and Z. Luthey-Schulten
- *Seminar* presented virtually for the JCVI Minimal Workshop 2022, Sept. 2022.

Towards deciphering the influence of genome architecture in a minimized bacterial genome *IPoLs Meeting 2022*
- T. A. Brier, P. Venepally, J.I. Glass, and Z. Luthey-Schulten
- *Seminar* presented at the annual International Physics of Living Systems Meeting Jun. 2022 in Montepellier, France.

Deciphering the influence of genome architecture in a minimized bacterial genome *American Physical Society Meeting 2022*
- T. A. Brier, P. Venepally, J.I. Glass, and Z. Luthey-Schulten
- *Seminar* presented at the annual American Physical Society Meeting Mar. 2022 in Chicago, IL.

Genome architecture in Syn1.0 and the minimal cell, Syn3A *JCVI Minimal Cell Workshop 2021*
- T. A. Brier, P. Venepally, J.I. Glass, and Z. Luthey-Schulten
- *Seminar* presented virtually for the JCVI Minimal Cell Workshop 2021 Sept. 2021

Modeling the nucleotide metabolic network of a genetically minimal cell *Biophysical Society Meeting 2020*
- T. A. Brier, D.M. Bianchi, Z.R. Thornburg, M.C.R. Melo, M. Breuer, H.O. Smith, C.A. Hutchison III, K.S. Wise, J.I. Glass, and Z. Luthey-Schulten.
- *Poster* presented at the annual Biophysical Society Meeting Feb. 2020 in San Deigo, CA.

Modeling the impact of point mutations on the regulatory potency of the small RNA SgrS *Biophysical Society Meeting 2019*
- T. A. Brier, D.M. Bianchi, A. Poddar, M.S. Azam, C.K. Vanderpool, T. Ha, and Z. Luthey-Schulten
- *Poster* presented at the annual Biophysical Society Meeting Mar. 2019 in Baltimore, MD.

Developing a method to identify ligand binding sites in proteins using molecular dynamics *REU Poster Session 2016*
- T. A. Brier, P.T. Lake, and M. McCullagh
- *Poster* presented at Colorado State University Research for Undergraduates Experience poster session Aug. 2016 in Fort Collins, CO.

Molecular simulations of type IV pilin subunits from three organisms in a lipid *American Chemical Society Meeting 2016*
- T. A. Brier and J.L. Baker
- *Poster* presented at the American Chemical Society meeting Mar. 2016 in San Diego, CA.

Stabilizing effect of a bacterial lipid membrane on type IV pilin subunits *MUSE Poster Session 2015*
- T. A. Brier and J.L. Baker
- *Poster* presented at the Mentored Undergraduate Summer Experience poster session hosted at TCNJ Sept. 2015 in Ewing, NJ.

Technical Skills

Programming : Python, MATLAB, Bash, R, Tcl, LaTeX, C/C++, CUDA, HTML
Tools : Unix/Linux, MacOS, Windows, AWS, SVN, Git, SSH, Docker, Apptainer, slurm, Jupyter, VScode, MARTINI CG, NVIDIA DGX
Software : pandas, matplotlib, seaborn, numpy, scipy, biopython, cobra, HTSeq, Guppy, minimap2, PyTorch, sklearn, HDF5, VMD, MAFFT, Clustal, BLAST, deepTools, SAMtools, GROMACS, AMBERMD, NAMD, AlphaFold2
Theoretical Training : *Mathematics* — Probability Theory, Stochastic Processes, Information Theory, Numerical Analysis, Linear Algebra, ODEs | *Science & Engineering* — Biophysics, Systems Biology, Bioinformatics, Molecular Dynamics, Equil. and Nonequil. Statistical Physics and Thermodynamics, Quantum Mechanics, Chemical Kinetics

Outreach and Activities

Luthey-Schulten Group Server Administrator | The Luthey-Schulten Group at UIUC *Winter 2022 - Summer 2024*
- Maintained research groups DGX and high-performance supercomputer systems.
- Established usage protocols for the systems, and then taught them to other groups members.
- Installed containerized (Docker and Apptainer) versions of group software to greatly improve computational performance.

Student Faculty Hiring Committee Member | Volunteer Organization at UIUC *Fall 2020, Fall 2022 - Spring 2024*
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Sloan UCEM Mini-Conference | Volunteer Organization at UIUC *Winter 2018 - Winter 2023*
- Attended a professional development, networking, and research poster session event for the Sloan fellows through the University Center of Exemplary Mentoring. Learned about graduate studies planning along with incorporating diversity at the graduate level. Hosted at the UIUC. Attended January 2018, 2019, 2020, 2021, 2022, 2023.

SEBA Mentor | Volunteer Organization at UIUC *October 2022*

- St. Elmo Brady Academy Performed demos for local middle school students focusing on promoting science to youth and teaching them about basic concepts such as luminescence.

Google Chicago PhD Summit Participant | Volunteer Organization at UIUC *Fall 2019*

- Accepted and attended an event highlighting opportunities at Google for PhD recipients in computer science related fields.

Poster Judge for ACS Undergrad Conference *Fall 2019*

- Served as a graduate student judge for the ACS Undergraduate conference held at the University of Illinois at Urbana-Champaign

Young Scholars Summer Research Program Mentor Facilitator | Volunteer Organization at UIUC *Summer 2019*

- Served in a more senior role in the Young Scholars Summer Research program this time working with other mentors and their students to provide support throughout the program.
- Advised two sets of mentor-mentee pairs throughout the program.

Physical Chemistry Student Seminar Selection Committee Member | Volunteer Organization at UIUC *Fall 2019*

- Served on panel of students responsible for choosing and hosting guest speakers.
- Presented brief research presentations to visiting faculty during lunch with fellow committee members.

Institute on Teaching and Mentoring Conference | Alfred P. Sloan Foundation at UIUC *October 2018*

- Attended a multi-day event focused on spreading research, networking, and mentoring/teaching targeted towards under-represented graduate students.
- Learned strategies for success at the graduate student level but also in roles as faculty members

Young Scholars Summer Research Program Mentor | CPLC at UIUC *Summer 2018*

- Mentored a student from a local area high school student through an eight-week research program tailored to teach roughly 30 students about research and the skills necessary to be a productive scientist.
- Advised the student on a project, which culminated in a poster presentation at the end of the program.
- Recognized as an *outstanding mentor* by the program.
- by the NSF Center for the Physics of Living Cells Performed demos for local middle school students focusing on promoting science to youth and teaching them about basic concepts such as luminescence.

Encouraging Tomorrow Chemist Mentor | Volunteer Organization at UIUC *Spring 2018*

- Performed demos for local middle school students focusing on promoting science to youth and teaching them about basic concepts such as luminescence.