# Noah Trebesch

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## **NSF Graduate Research Fellow**

Emad Tajkhorshid Research Group (Computational Structural Biology and Molecular Biophysics Group) Beckman Institute for Advanced Science & Technology University of Illinois at Urbana-Champaign 3109 Beckman Institute, 405 N Matthews Ave Urbana, IL 61801

#### PhD Candidate

Center for Biophysics and Quantitative Biology University of Illinois at Urbana-Champaign 318C Roger Adams Laboratory, 600 S Mathews Ave Urbana, IL 61801

> Nov, 2016 Mar, 2016 Apr, 2015

Jan, 2014

## Education

University of	of Illinois at Urbana-Champaign	, Center for Biophysics and Quantitative Biol	ogy (Urbana, IL)
Degree:	PhD in Biophysics and Computational Biology		Dec, 2023 (Expected)
University o	of Minnesota – Twin Cities, Colle	ege of Science & Engineering (Minneapolis, I	MN)
Degrees:	BS in Physics	Emphasis: Biological Physics	May, 2014
	BS in Computer Science	Computational Science	May, 2014
Thesis:	"A Computational Method for Investigating Bifurcations in Oscillatory Biochemical Reaction Netwo		ochemical Reaction Networks"
	Distin	ctions, Awards, and Associations	
University of	of Illinois at Urbana-Champaign	, Center for Biophysics and Quantitative Biol	ogy (Urbana, IL)
Distinctions			
Beckman Institute Student Researcher of the Week			Nov, 2018
Awards			
Travel Grant, Department of Biochemistry		Nov, 2016; Nov, 2019	
	•		May, 2022; Nov, 2022
Travel Award, Biophysical Society		Nov, 2018	

• -	Travel Grant, Graduate College
•	NSF Graduate Research Fellowship Program (GRFP) Awardee
•	DOE Computational Science Graduate Fellowship (CSGF) Honorable Mention

- Hans Frauenfelder Graduate Award, Center for Biophysics and Quantitative Biology
   Associations
- Biophysical Society
   NIH Resource for Macromolecular Modeling and Visualization
   Out in STEM (oSTEM) at Illinois, Internal Vice President (Apr, 2016-Aug, 2018)
   American Physical Society
   Membrane Protein Structural Dynamics Consortium (MPSDC), NIH/NIGMS
   Jan, 2015-Present
   Jan, 2015-Present

## **University of Minnesota – Twin Cities, College of Science & Engineering (Minneapolis, MN)** *Distinctions*

Cum Laude Latin Honors in Physics, University Honors Program (UHP)	May, 2014
Dean's List, College of Science & Engineering	Fall, 2011; Spring, 2014
Dean's List, College of Continuing Education	Fall, 2008-Spring, 2010
Awards	
<ul> <li>John Tate Memorial Scholarship, College of Science &amp; Engineering</li> </ul>	May, 2012
Technical Leadership Challenge Scholarship, College of Science & Engineering	May, 2012
<ul> <li>Lando Scholarship, Department of Computer Science &amp; Engineering</li> </ul>	May, 2012

- Harry and Viola St. Cyr Scholarship for Summer Research, School of Physics and Astronomy Apr, 2012
- Ruby Hackett and Weldon Jones Scholarship, University of Minnesota Twin Cities
   Mar, 2010

- National Merit Scholarship Qualifying Test (NMSQT) Special Scholarship, 3M Company
- Woodbury Chamber of Commerce Scholarship •
- Cans for College Scholarship, Woodbury Veterans of Foreign Wars (VFW) Post 9042 Associations
- University Honors Program (UHP)
- Undergraduate Research Opportunities Program (UROP)

Research

#### University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science & Technology (Urbana, IL) Sept, 2014-Present

Position: Research Assistant

- PI: Professor Emad Tajkhorshid
- Developing software to atomistically model, visualize, and simulate cell-scale membrane structures derived from experimental 3D data.
  - o xMAS (Experimentally-Derived Membranes of Arbitrary Shape) Builder
  - Analyzes 3D meshes derived from techniques like electron microscopy to determine placement, orientation, and number of lipid molecules.
  - Optimizes lipid placement using an MD-based technique, builds atomistic model using a set of lipid conformation libraries, and eliminates complex lipid clashes using an energy minimization simulation technique.
  - Current application is a Terasaki ramp, a structural motif from endoplasmic reticula with a complex helicoidal structure like that of a parking ramp.
  - Models allow the interplay between atomic-scale biochemistry and cellscale biophysics to be probed for the first time.
- Structurally elucidating and thermodynamically characterizing the mechanism of membrane transporters through computational techniques.
  - Current transporters include NaCT, VcINDY, and LaINDY.
  - Uses nonequilibrium driven molecular dynamics (MD), string method with swarms of trajectories (SMwST), bias-exchange umbrella sampling (BEUS), and other advanced parallel computational techniques that require the use of supercomputers.
  - Structural modeling and bioinformatics techniques also utilized.
  - Provides key insight to biomedical researchers developing drugs targeting transporters and synthetic bioengineers developing custom biomachines.

## University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science & Technology (Urbana, IL)

PI: Professor Klaus Schulten

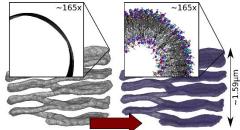
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Position: Research Assistant

- Sought to computationally elucidate the mechanism by which YidC inserts the polypeptide chain synthesized by the ribosome into the membrane.
- Used nonequilibrium molecular dynamics to drive nascent chain insertion and molecular dynamics flexible fitting (MDFF) to model the ribosomal exit tunnel in preliminary simulations.
- Ran simulations with the full ribosome that contained ~5.6 million atoms.
- Designed, ran, and analyzed simulations in collaboration with Rezvan Shahoei and Dr. Abhishek Singharoy.

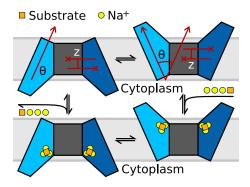


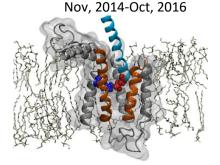
Sept, 2010-May, 2014 Sept, 2012-Jan, 2013



Experimental Mesh

Atomistic Model





#### University of Minnesota – Twin Cities, School of Physics and Astronomy (Minneapolis, MN)

Position: Undergraduate Researcher PI: Professor Jorge Viñals

- Developed a parallel C++ program that modified the Gillespie Stochastic Simulation Algorithm (SSA) to simulate biochemical systems forward and backward in time.
- Designed the program to numerically investigate the bifurcation points and transience that typically govern the behavior of gene oscillators.
- Applied the program as proof of concept to the continuous and discontinuous Schlögl models, whose deterministic and stochastic behavior is well known.
- Represents the first step required to design synthetic gene oscillators that can output ideal, tunable signals.

#### University of Minnesota – Twin Cities, Chemical Engineering & Material Science Department (Minneapolis, MN) *Position:* Undergraduate Researcher *PI:* Professor Yiannis Kaznessis Jun, 2012-Sept, 2

- Developed and refined Hy3S (Hybrid Stochastic Simulation for Supercomputers), a ~5300 line Fortran program used to simulate systems of biochemical reactions accurately and efficiently using a multiscale SSA.
- Optimized and updated the source code to drastically restructure the program, fix bugs, improve performance, and make future development easier.
- Program is now more stable and runs faster, and researchers who use the program can more easily specialize it to suit their specific needs.

#### 3M Company, Display & Graphics Film Lab (Maplewood, MN)

Position: Technical Aide

#### PI: Steve Johnson

- Worked in a research and development engineering lab which innovates new multilayer optical films to be used in various commercial applications.
- Took and analyzed physical and optical data from dozens of different film tests (tensile strength, delamination, refractive indices, colorimetry, spectrophotometry, transmittance, haze, clarity, etc.).
- Data and analysis helped my supervisor and his colleagues determine which projects to pursue and how to refine their work to produce higher quality films with novel applications.

#### University of Minnesota – Twin Cities, School of Physics and Astronomy (Minneapolis, MN)

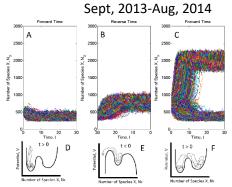
- *Position:* Research Team Member *PI:* Professor J. Woods Halley
  Used magnetite electrodes in an attempt to electrolyze water more efficiently.
- Took and analyzed data in the form of electrical current-voltage curves.
- Performed background research into refining and enhancing the experiment.

# Research (Short-Term Experiences)

# University of Illinois at Urbana-Champaign, Department of Chemistry (Urbana, IL)

Position: Rotation Research Assistant PI: Professor Sharon Hammes-Schiffer

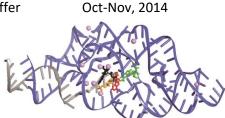
- Used quantum mechanical/molecular mechanical (QM/MM) simulation techniques to investigate the mechanism of glmS ribozyme catalysis.
- Built a parallel C++ program for classical molecular dynamics simulations of pure elemental liquids from scratch.
- Built a Python script to perform a Hartree-Fock Self-Consistent Field STO-G3 energy calculation.



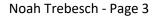
Jun, 2012-Sept, 2013 BMC-Example2-2-1 New Code: gfortran New Code: ifort Old Code: ifort







Aug, 2010-Jun, 2012



#### University of Minnesota – Twin Cities, School of Physics and Astronomy (Minneapolis, MN)

Position: Student

#### Mentor/Instructor: Professor Clem Pryke

- Attempted to replicate in collaboration with Ben Freund the experiment and results of Y. Han *et al. Science*. **314**:626 (2006)., in which the Brownian motion of microscopic ellipsoidal particles was quantitatively studied.
- Created ellipsoidal particles from spherical polystyrene particles, prepared slides to simulate quasi-two dimensional confinement, and filmed the particles using video light microscopy.
- Wrote an image processing script in MATLAB to track the orientation and position of the filmed particles through time and confirmed that the experimental data matched theoretical expectations.
- Results contribute to the understanding of the Brownian motion experienced by biological macromolecules.

#### University of Minnesota – Twin Cities, Department of Computer Science & Engineering (Minneapolis, MN)

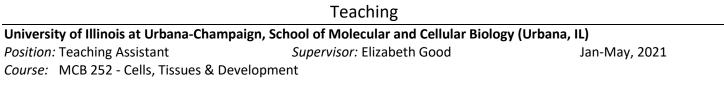
Position: Student Instructor: Professor Vicky Interrante

- Developed a C++ program from scratch for visualizing molecules in 3D.
- Implemented space filling, ball-and-stick, and stick models with numerous display options using The Visualization Toolkit, as well as an interface to read data from SDF files available from PubChem.

#### University of Minnesota – Twin Cities, Department of Computer Science & Engineering (Minneapolis, MN)

Position: Student

- Attempted to use Gaussian kernel ridge regression to predict the boiling points of molecular compounds based on their composition and structure.
- Results can be used to gauge how successful this technique might be for predicting other chemical information from composition and structure.
- Results have applications in pharmaceutical drug design and discovery.



#### NIH Center for Macromolecular Modeling and Bioinformatics (Urbana, IL)

Position: Teaching AssistantSupervisor: Professor Emad TajkhorshidApr, 2015-Oct, 2021Course:Theoretical and Computational Biophysics Group (TCBG) "Hands-on" Workshop on Computational BiophysicsVirtual: Oct. 2020; Oct. 2021

- Virtual; Oct, 2020; Oct, 2021
- University of Illinois at Urbana-Champaign, Urbana, IL; Apr, 2015; Oct, 2016; Apr, 2017
- University of California, Berkeley, Berkeley, CA; Aug, 2015

Course: TCBG "Hands-on" Workshop on Enhanced Sampling and Free-Energy Calculation

• University of Illinois at Urbana-Champaign, Urbana, IL; Sept, 2017

## University of Illinois at Urbana-Champaign, Department of Physics (Urbana, IL)

Position: Laboratory Teaching AssistantSupervisor: Professor Munir NayfehJan-May, 2016Course:PHYS 101 – College Physics: Mechanics and HeatJan-May, 2016

## Volunteering and Service

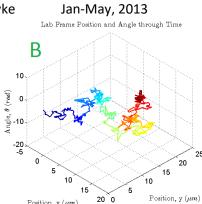
# The Trevor Project (Virtual)

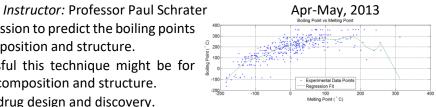
Position: Volunteer

Contact: info@thetrevorproject.org

Aug, 2020-Present

- The Trevor Project is the leading national organization providing crisis intervention and suicide prevention services to LGBT+ youth.
- Performed various tasks to support the mission of the Trevor Project. (3 hours/week)





Mar-May, 2013

#### Member Committee, oSTEM at Illinois (Urbana, IL)

Position: Member, Internal Vice President *Contact:* Joy Bryant

- oSTEM is a professional association for LGBT+ people in the STEM community, composed primarily of student chapters at universities across the United States and around the world.
- Responsible for coordinating the outreach activities of oSTEM and for planning some of the weekly oSTEM meetings. (1 hour/week)
- Designed and gave presentations during oSTEM meetings on what undergraduate research is and how to get involved and on how to design research abstracts/posters/presentations.
- Helped create a presentation for local high schools about being LGBT+ in STEM in college.
- Helped prepare the 2016, 2017, and 2018 oSTEM exhibits for the UIUC Engineering Open House, which is designed to engage the local public (especially elementary, middle, and high school students) with STEM.
- Hosted an event where UIUC professors shared their experiences being LGBT+ in their careers.

## Urbana Middle School (Urbana, IL)

Position: Volunteer Tutor

- Supervisor: Barbara Linder • Served as an in-classroom tutor in a sixth grade class for general science taught by Theresa Feller and a seventh grade class for mathematics taught by Grace Householder. (2 hours/week; Sept, 2015-May, 2016)
- Served as an in-classroom tutor for the summer school for grades six through eight in nonfiction and fiction literature classes taught by Martina Connell and Katie Skarzynski, respectively. (8 hours/week; Jun, 2015)

#### University of Illinois at Urbana-Champaign, Beckman Institute for Advanced Science & Technology (Urbana, IL)

Position: Research Assistant Supervisor: Professor Emad Tajkhorshid Feb, 2015-May, 2015

- Developed educational materials with the Tajkhorshid research group that use engineering techniques to facilitate deeper biological and biochemical understanding in the classroom. (1 hour/week)
- Materials will be used in advanced undergraduate biology and biochemistry courses.
- My lesson demonstrates the structure and stability of different protein secondary structures by using driven molecular dynamics simulations to pull these structures apart.

## Washington County Public Library (Woodbury, MN)

*Position:* Volunteer

Supervisor: Marty Hoekstra

Jun, 2007-Aug, 2010

- Shelved books and performed various administrative tasks to help keep the library running. (1-4 hours/week; Sept, 2007-Aug, 2010)
- Assisted with a summer program that encouraged pre-teens to read. (2 hours/week; Jun-Aug, 2007)

## **Publications and Presentations**

#### University of Illinois at Urbana-Champaign, Center for Biophysics and Quantitative Biology (Urbana, IL)

*Publications (\*Equal Contribution, <sup>†</sup>Corresponding Author)* 

- N. Trebesch and E. Tajkhorshid<sup>+</sup>. "xMAS Builder: Software for Generating Atomistic Models of Realistic Cellular Membranes for Molecular Dynamics." (In Preparation).
- <u>N. Trebesch</u> and E. Tajkhorshid<sup>+</sup>. "Structure Reveals Homology in Elevator Transporters." (Submitted).
- A. Trifan\*, D. Gorgun\*, M. Salim\*, Z. Li\*, A. Brace\*, M. Zvyagin\*, H. Ma\*, A. Clyde, D. Clark, D. J. Hardy, T. Burnley, L. Huang, J. McCalpin, M. Emani, H. Yoo, J. Yin, A. Tsaris, V. Subbiah, T. Raza, J. Liu, N. Trebesch, G. Wells, V. Mysore, T. Gibbs, J. Phillips, S. C. Chennubhotla, I. Foster, R. Stevens, A. Anandkumar<sup>†</sup>, V. Vishwanath<sup>†</sup>, J. E. Stone<sup>†</sup>, E. Tajkhorshid<sup>†</sup>, S. A. Harris<sup>†</sup>, and A. Ramanathan<sup>†</sup>. "Intelligent resolution: Integrating Cryo-EM with AI-driven multi-resolution simulations to observe the severe acute respiratory syndrome coronavirus-2 replication-transcription machinery in action." International Journal of High-Performance Computing Applications. 36:5-6, 603-623 (2022).
- D. B. Sauer, N. Trebesch, J. J. Marden, N. Cocco, J. Song, A. Koide, S. Koide, E. Tajkhorshid<sup>†</sup>, and D.-N. Wang<sup>†</sup>. "Structural basis for the reaction cycle of DASS dicarboxylate transporters." *eLife*. 9, e61350 (2020).
- T. Jiang, P.-C. Wen, N. Trebesch, Z. Zhao, S. Pant, K. Kapoor, M. Shekhar, and E. Tajkhorshid<sup>+</sup>. "Computational Dissection of Membrane Transport at a Microscopic Level." Trends in Biochemical Sciences. 45:3, 202-216 (2020).
- P.-C. Wen\*, P. Mahinthichaichan\*, N. Trebesch, T. Jiang, Z. Zhao, E. Shinn, Y. Wang, M. Shekhar, K. Kapoor, C. K. Chan, and E. Tajkhorshid<sup>+</sup>. "Microscopic View of Lipids and Their Diverse Biological Functions." Current Opinion in Structural Biology. 51, 177-186 (2018).

Oct, 2015-May, 2018

Jun, 2015-May, 2016

- <u>N. Trebesch</u>, J. V. Vermaas, and E. Tajkhorshid<sup>†</sup>. "Computational Characterization of Molecular Mechanisms of Membrane Transporter Function." *Computational Biophysics of Membrane Proteins*. C. Domene, Ed. 197-236 (Royal Society of Chemistry, Cambridge, 2016).
- J. V. Vermaas, <u>N. Trebesch</u>, C. G. Mayne, S. Thangapandian, M. Shekhar, P. Mahinthichaichan, J. L. Baylon, T. Jiang, Y. Wang, M. P. Muller, E. Shinn, Z. Zhao, P.-C. Wen, and E. Tajkhorshid<sup>†</sup>. "Microscopic Characterization of Membrane Transporter Function by In Silico Modeling and Simulation." *Methods in Enzymology: Computational Approaches for Studying Enzyme Mechanism Part B*. G. E. Voth, Ed. **578**:16 (2016).

*Oral Presentations (\*Presenting Author, <sup>+</sup>Session Co-Chair)* 

- <u>N. Trebesch</u>\* and E. Tajkhorshid "Structure Reveals Homology in Elevator and Rocking Bundle Transporters." *Gordon Research Conference (GRC) on Mechanisms of Membrane Transport*. Les Diablerets, Switzerland (20 Jun 2023).
- <u>N. Trebesch</u>\*, D. B. Sauer, D.-N. Wang, and E. Tajkhorshid. "Mechanistic Insights from Molecular Dynamics Simulations of Large-Scale Conformational Transitions in the INDY Transport Cycle." *Biophysical Society 65th Annual Meeting*. Virtual (22 Feb 2021). (Video Recording: https://bit.ly/3qtFBDU)
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Multibillion Atom Molecular Dynamics Simulations of Cellular Membranes." *American Physical Society (APS) March Meeting 2020*. Virtual (2 Mar 2020).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *School of Molecular and Cellular Biology Retreat*. Champaign, IL (6 Sep 2019).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Incorporating Proteins into Geometrically Complex, Cell-Scale Membrane Models." *Blue Waters Symposium 2019*. Sunriver, OR (5 Jun 2019). (Video Recording: https://bit.ly/2n66SRA)
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Modeling and Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures with xMAS Builder." *8th Annual oSTEM National Conference*. Houston, TX (18 Nov 2018).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *Beckman Institute Graduate Student Seminar*. Urbana, IL (7 Nov 2018).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Modeling and Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures with xMAS Builder." *NAMD Developer Workshop*. Urbana, IL (12 Jun 2018).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *Blue Waters Symposium 2018*. Sunriver, OR (6 Jun 2018). (Video Recording: https://bit.ly/2KOCbXj)
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *Biophysical Society 62nd Annual Meeting*. San Francisco, CA (21 Feb 2018).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Modeling and Characterizing the Structural and Thermodynamic Aspects of the Elevator Transport Mechanism of VcINDY." *Poster Rapid Fire Session, Membrane Protein Structural Dynamics Consortium (MPSDC) 2017 Annual Meeting.* Lemont, IL (10 Nov 2017).
- <u>N. Trebesch</u>\*. "Atomistic Modeling and Simulation of Organelle-Scale Membrane Structures of Arbitrary Size, Lipid Composition, and Geometric Complexity." *Center for the Physics of Living Cells/Center for Biophysics and Quantitative Biology Graduate Student and Postdoc Symposium*. Urbana, IL (19 Sept 2017). (Voted Third Best Speaker)
- <u>N. Trebesch</u>\*. "Atomistic Modeling and Simulation of Cell-Scale Membrane Structures with xMAS Builder." *NAMD Developer Workshop*. Chicago, IL (22 May 2017).
- <u>N. Trebesch</u><sup>\*†</sup> and E. Tajkhorshid. "Atomistic Modeling of Organelle-Scale Membrane Structures of Arbitrary Size, Lipid Composition, and Geometric Complexity." *Biophysical Society 61st Annual Meeting*. New Orleans, LA (15 Feb 2017).
- M. Moradi, J. Li, P.-C. Wen, S. Thangapandian, J. Vermaas, D. Sabri Dashti, <u>N. Trebesch</u>, and E. Tajkhorshid\*. "Visualizing complex functional motions of membrane transporters at an atomic resolution." *10th EBSA European Biophysics Congress*. Dresden, Germany (18-22 Jul 2015).
- <u>N. Trebesch</u>\*. "Elevator Mode of Transport in VcINDY, a Bacterial Na-Coupled Transporter." Computational Modeling Mini-Symposium, Membrane Protein Structural Dynamics Consortium (MPSDC) 2015 Annual Meeting. Chicago, IL (29 Apr 2015).

Posters (\*Presenting Author)

- <u>N. Trebesch</u>\* and E. Tajkhorshid "Structure Reveals Homology in Elevator and Rocking Bundle Transporters."
  - Gordon Research Conference (GRC) on Mechanisms of Membrane Transport. Les Diablerets, Switzerland (22 Jun 2023).
  - Gordon Research Seminar (GRS) on Mechanisms of Membrane Transport. Les Diablerets, Switzerland (18 Jun 2023).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "The Homology of Elevator and Rocking Bundle Transporters." *Biophysical Society* 67th Annual Meeting. San Diego, CA (21 Feb 2023).

- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Multibillion Atom Molecular Dynamics Simulations of Complex Cellular Membranes." *Biophysical Society Thematic Meeting: Biophysics at the Dawn of Exascale Computers*. Hamburg, Germany (18 May 2022).
- <u>N. Trebesch</u>\* and E. Tajkhorhsid. "Structural Phylogenetics Suggest Evolutionary Relationships Exist Between Most Elevator Transporters." *Biophysical Society 66th Annual Meeting*. San Francisco, CA (21 Feb 2022).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Embracing Biological Complexity in Atomistic Simulations of Cellular Membranes." *Biophysical Society 64th Annual Meeting*. San Diego, CA (16 Feb 2020).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Incorporating Proteins into Geometrically Complex, Cell-Scale Membrane Models for Molecular Dynamics Simulations."
  - 2019 Oak Ridge Leadership Computing Facility (OLCF) User Meeting. Oak Ridge, TN (21 May 2019).
  - o Biophysical Society 63rd Annual Meeting. Baltimore, MD (4 Mar 2019).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Modeling and Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures with xMAS Builder."
  - o 8th Annual oSTEM National Conference. Houston, TX (17 Nov 2018).
  - o Illinois Biophysics Society Biophysics Graduate Research and Networking Symposium. Urbana, IL (30 Oct 2018).
  - o UIUC New Graduate Student Welcome Reception. Urbana, IL (27 Aug 2018).
  - 2018 Oak Ridge Leadership Computing Facility (OLCF) User Meeting. Oak Ridge, TN (15 May 2018).
- <u>N. Trebesch</u>\* and E. Tajkhorshid. "Modeling and Characterizing the Structural and Thermodynamic Aspects of the Elevator Transport Mechanism of VcINDY."
  - o 7th Annual oSTEM National Conference. Chicago, IL (18 Nov 2017).
  - Membrane Protein Structural Dynamics Consortium (MPSDC) 2017 Annual Meeting. Lemont, IL (10-12 Nov 2017).
  - o Illinois Biophysics Society Biophysics Graduate Research and Networking Symposium. Urbana, IL (23 Oct 2017).
  - o UIUC New Graduate Student Welcome Reception. Urbana, IL (28 Aug 2017).
  - o Gordon Research Conference (GRC) on Mechanisms of Membrane Transport. New London, NH (28-29 Jun 2017).
- <u>N. Trebesch</u>\*, J. V. Vermaas, and E. Tajkhorshid. "A Molecular Dynamics Based Model of the Outward-Facing State and Transport Mechanism of the Human NaCT Homolog VcINDY."
  - 6th Annual oSTEM National Conference. Denver, CO (12 Nov 2016).
  - Biophysical Society 60th Annual Meeting. Los Angeles, CA (2 Mar 2016).
- R. Shahoei, <u>N. Trebesch</u>\*, A. Singharoy, and K. Schulten. "Structure and function of YidC, an insertase that channels newly synthesized proteins into the cell membrane." *Biophysical Society 60th Annual Meeting*. Los Angeles, CA (29 Feb 2016).
- R. Shahoei\*, A. Singharoy, <u>N. Trebesch</u>, and K. Schulten. "Structure and function of YidC, an insertase that channels newly synthesized proteins into the cell membrane." *International Physics of Living Systems (iPoLS) Network 2015 Annual Meeting*. Arlington, VA (19 Jul 2015).
- <u>N. Trebesch</u>\*, P.-C. Wen, M. Moradi, and E. Tajkhorshid. "Computational Characterization of the Transport Mechanism of the Folate ECF Membrane Transporter."
  - *Membrane Protein Structural Dynamics Consortium (MPSDC) 2015 Annual Meeting*. Chicago, IL (30 Apr 2015).
  - *Biophysical Society 59th Annual Meeting*. Baltimore, MD (9 Feb 2015).

#### **University of Minnesota – Twin Cities, College of Science & Engineering (Minneapolis, MN)** *Publications*

- <u>N. Trebesch</u> and J. Viñals. "A Computational Method for Investigating Bifurcations in Oscillatory Biochemical Reaction Networks." *University Honors Program Theses*. (2014). <a href="https://github.com/noahtreb/rxn-sys-sim">https://github.com/noahtreb/rxn-sys-sim</a>.
- <u>N. Trebesch</u>. "Updates and Improvements to Hy3S." *Hy3S Hybrid Stochastic Simulation for Supercomputers*. (2013). <a href="http://sourceforge.net/projects/hysss/files/Hy3S%20Simulation%20Programs/v2.0.1/>">http://sourceforge.net/projects/hysss/files/Hy3S%20Simulation%20Programs/v2.0.1/</a>.
- <u>N. Trebesch</u> and B. Freund. "Brownian Motion of Ellipsoidal Particles." *Methods of Experimental Physics Projects*. (2013). <a href="https://wiki.umn.edu/MXP/BrownianMotionofNon-SphericalParticles">https://wiki.umn.edu/MXP/BrownianMotionofNon-SphericalParticles</a>.
- J. W. Halley, A. Schofield, and B. Berntson. "Use of magnetite as anode for electrolysis of water." *Journal of Applied Physics*. **111**:124911 (2012). (Acknowledgement).

Oral Presentations (\*Presenting Author)

 <u>N. Trebesch</u>\*. "A Computational Method for Investigating Bifurcations in Oscillatory Biochemical Reaction Networks." University Honors Program (UHP) Thesis Defense. School of Physics and Astronomy, University of Minnesota – Twin Cities, Minneapolis, MN (23 Apr 2014).

#### Posters (\*Presenting Author)

• <u>N. Trebesch</u>\* and B. Freund\*. "Brownian Motion of Ellipsoidal Particles." *Methods of Experimental Physics Poster Session*. School of Physics and Astronomy, University of Minnesota – Twin Cities, Minneapolis, MN (10 May 2013).