Noah Trebesch

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Postdoctoral Research Associate
Emad Tajkhorshid Research Group
(Computational Structural Biology and Molecular Biophysics Group)
Beckman Institute for Advanced Science & Technology
University of Illinois Urbana-Champaign
3151 Beckman Institute, 405 N Matthews Ave, Urbana, IL 61801

Education

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

Degree:	PhD in Biophysics and Computational Biology	Dec 2023
Dissertation:	"Computational Investigations of the Structure, Function, and Evolution of Complex Membrane Systems"	

University of Minnesota – Twin Cities, College of Science & Engineering (Minneapolis, 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 Networks"		

Distinctions, Awards, and Associations

University of Illinois Urbana-Champaign, Beckman Institute for Advanced Science & Technology (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	Nov 2016
• NSF Graduate Research Fellowship Program (GRFP) Awardee	Mar 2016
• DOE Computational Science Graduate Fellowship (CSGF) Honorable Mention	Apr 2015
• Hans Frauenfelder Graduate Award, Center for Biophysics and Quantitative Biology	Jan 2014

Associations

• Biophysical Society	Jan 2015-Present
• NIH Resource for Macromolecular Modeling and Visualization	Jan 2015-Present
• American Physical Society	Oct 2019-Dec 2020
• Membrane Protein Structural Dynamics Consortium (MPSDC), NIH/NIGMS	Jan 2015-Aug 2019
• Out in STEM (oSTEM) at Illinois, Internal Vice President (Apr 2016-Aug 2018)	May 2015-Aug 2018

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

• John Tate Memorial Scholarship, College of Science & Engineering	May 2012
• Technical Leadership Challenge Scholarship, College of Science & Engineering	May 2012
• Lando Scholarship, Department of Computer Science & Engineering	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	Spring 2010

- Woodbury Chamber of Commerce Scholarship   Spring 2010
- Cans for College Scholarship, Woodbury Veterans of Foreign Wars (VFW) Post 9042   Spring 2010

Associations
- University Honors Program (UHP)   Sep 2010-May 2014
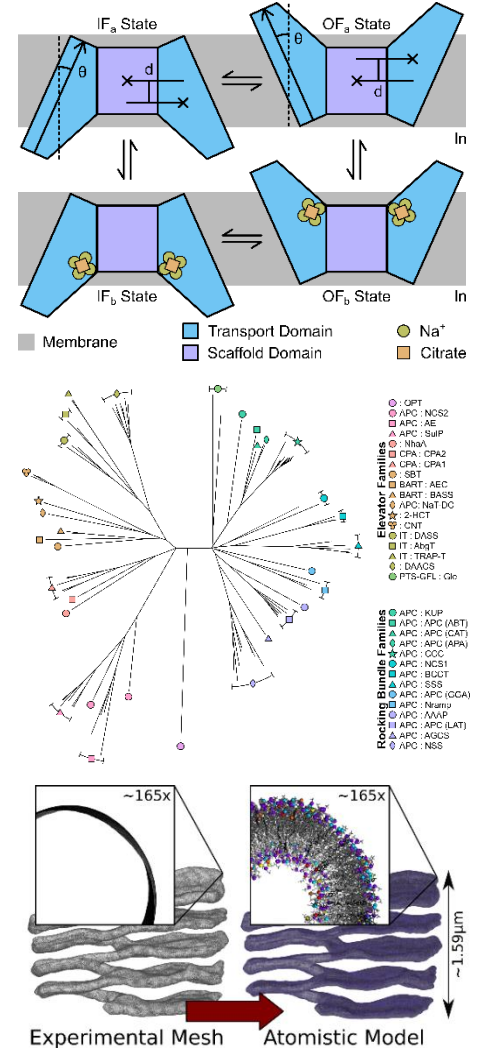- Undergraduate Research Opportunities Program (UROP)   Sep 2012-Jan 2013

Research

University of Illinois Urbana-Champaign, Beckman Institute for Advanced Science & Technology (Urbana, IL)
Position: Research Associate   *PI:* Professor Emad Tajkhorshid   Sep 2014-Present

- Structurally and thermodynamically characterizing transporter mechanisms using advanced molecular dynamics (MD) simulation techniques.
  - Current transporters include NaCT, VcINDY, and LaINDY.
  - Uses collective variables, driven MD simulations, the string method with swarms of trajectories (SMwST), bias-exchange umbrella sampling (BEUS), and the weighted histogram analysis method (WHAM).
  - Also utilizes structural modeling and bioinformatics techniques.
  - Provides key insight to biomedical researchers developing drugs targeting transporters and synthetic bioengineers developing custom biomachines.
- Investigating the evolutionary relationships between elevator and rocking bundle transporters using comparative structural analyses.
  - Involves developing from scratch a new computational framework to perform topology-corrected structural comparisons between transporters.
  - Also involves generating a phylogenetic tree to enable visualization of the evolutionary relationships between transporter families.
  - Constitutes a powerful new evolutionary context in which the fundamental similarities and differences between elevator and rocking bundle transporters and their mechanisms can be investigated and understood.
- Developing software to atomistically model, visualize, and simulate cell-scale membrane structures derived from experimental data.
  - xMAS (E**x**perimentally-Derived **M**embranes of **A**rbitrary **S**hape) 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 models 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 cell-scale biophysics to be probed for the first time.

University of Illinois Urbana-Champaign, Beckman Institute for Advanced Science & Technology (Urbana, IL)
Position: Research Assistant   *PI:* Professor Klaus Schulten   Nov 2014-Oct 2016

- Sought to computationally elucidate the mechanism by which YidC inserts the polypeptide chain synthesized by the ribosome into the membrane.
- Used driven MD to induce 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 Abhi Singharoy.
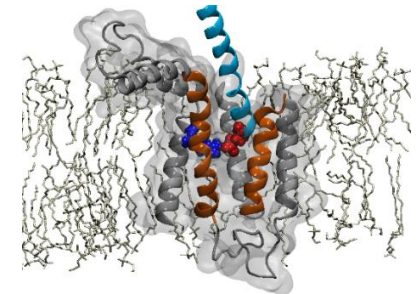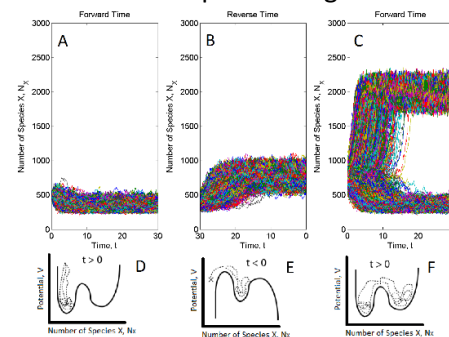
University of Minnesota – Twin Cities, School of Physics and Astronomy (Minneapolis, MN)
Position: Undergraduate Researcher   *PI:* Professor Jorge Viñals   Sep 2013-Aug 2014

- 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-Sep 2013

- 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.
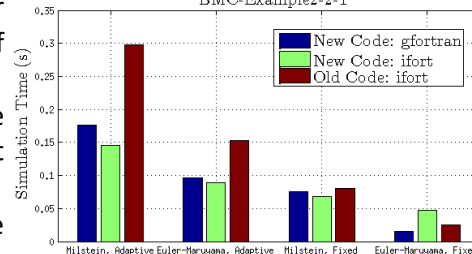
3M Company, Display & Graphics Film Lab (Maplewood, MN)
Position: Technical Aide   *PI:* Steve Johnson   Aug 2010-Jun 2012

- 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.
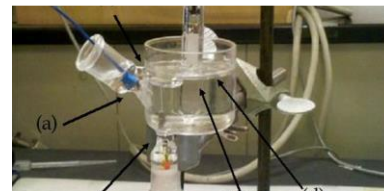
University of Minnesota – Twin Cities, School of Physics and Astronomy (Minneapolis, MN)
Position: Research Team Member   *PI:* Professor J. Woods Halley   Mar 2010-Jan 2011

- 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 Urbana-Champaign, Department of Chemistry (Urbana, IL)
Position: Rotation Research Assistant   *PI:* Professor Sharon Hammes-Schiffer   Oct-Nov 2014

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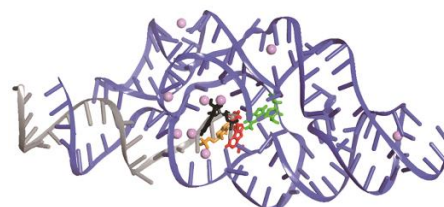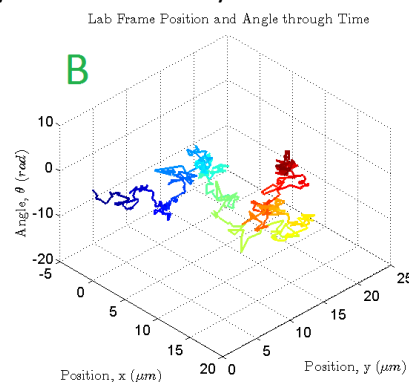
University of Minnesota – Twin Cities, School of Physics and Astronomy (Minneapolis, MN)

Position: Student   *Mentor/Instructor:* Professor Clem Pryke   Jan-May 2013

- 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   Mar-May 2013

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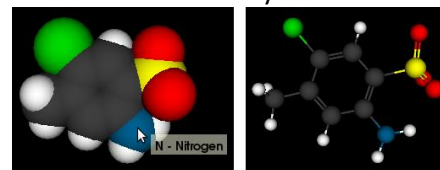
University of Minnesota – Twin Cities, Department of Computer Science & Engineering (Minneapolis, MN)

Position: Student   *Instructor:* Professor Paul Schrater   Apr-May 2013

- 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.
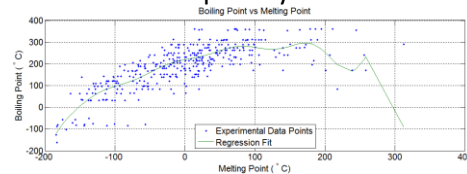
Teaching

NIH Resource for Macromolecular Modeling and Visualization (Urbana, IL)

Position: Teaching Assistant   *Supervisor:* Professor Emad Tajkhorshid   Apr 2015-Jun 2024

Course: Theoretical and Computational Biophysics Group (TCBG) "Hands-on" Workshop on Computational Biophysics

- Auburn University (Auburn, AL)	Jun 2024
- Virtual	Oct 2020, Oct 2021
- University of Illinois 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 Urbana-Champaign (Urbana, IL)	Sep 2017

University of Illinois Urbana-Champaign, School of Molecular and Cellular Biology (Urbana, IL)

Position: Teaching Assistant   *Supervisor:* Elizabeth Good   Jan-May 2021

Course: MCB 252 - Cells, Tissues & Development

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

Position: Laboratory Teaching Assistant   *Supervisor:* Professor Munir Nayfeh   Jan-May 2016

Course: PHYS 101 - College Physics: Mechanics and Heat

Volunteering and Service

The Trevor Project (Virtual)
Position: Trevor Volunteer Counselor   *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.
- Worked as a Volunteer Counselor to support the mission of the Trevor Project. (3 hours/week)

Member Committee, oSTEM at Illinois (Urbana, IL)
Position: Member, Internal Vice President   *Contact:* Joy Bryant   Oct 2015-May 2018
- 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   Jun 2015-May 2016
- 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, Sep 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 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, Sep 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 Urbana-Champaign, Beckman Institute for Advanced Science & Technology (Urbana, IL)
Publications (*Equal Contribution, †Corresponding Author)
- N. Trebesch and E. Tajkhorshid[†]. "xMAS Builder: Software for Generating Atomistic Models of Realistic Cellular Membranes for Molecular Dynamics." (In Preparation).
- N. Trebesch and E. Tajkhorshid[†]. "Structure Reveals Homology in Elevator Transporters." *Nature Communications*. (Under Revision). (Preprint: https://doi.org/10.1101/2023.06.14.544989)
- N. Trebesch[†]. "Computational Investigations of the Structure, Function, and Evolution of Complex Membrane Systems." *PhD Dissertation*. (2023). <https://hdl.handle.net/2142/122111>.
- 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[†], V. Vishwanath[†], J. E. Stone[†], E. Tajkhorshid[†],

S. A. Harris[†], and A. Ramanathan[†]. "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[†], and D.-N. Wang[†]. "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[†]. "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[†]. "Microscopic View of Lipids and Their Diverse Biological Functions." *Current Opinion in Structural Biology*. **51**, 177-186 (2018).
- N. Trebesch, J. V. Vermaas, and E. Tajkhorshid[†]. "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, N. Trebesch, 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[†]. "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, [†]Session Co-Chair)*

- N. Trebesch* and E. Tajkhorshid. "Capturing the Structural Dynamics and Energetics of the Large-Scale Elevator Transition of NaCT." *Biophysical Society 69th Annual Meeting*. Los Angeles, CA (16 Feb 2025).
- N. Trebesch* and A. Fakharzadeh*. "Using Advanced Molecular Dynamics Simulation Techniques to Characterize Large-Scale Conformational Transitions in Transporters." *Models, Inference & Algorithms (MIA) Initiative at the Broad Institute of MIT and Harvard*. Cambridge, MA (23 Oct 2024). (Video Recording: https://youtu.be/wT_fjRATbVY)
- N. Trebesch*. "Computational Investigations of the Structure, Function, and Evolution of Complex Membrane Systems." *PhD Defense*. Urbana, IL (1 Nov 2023).
- N. Trebesch* 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).
- N. Trebesch*, 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)
- N. Trebesch* and E. Tajkhorshid. "Multibillion Atom Molecular Dynamics Simulations of Cellular Membranes." *American Physical Society (APS) March Meeting 2020*. Virtual (2 Mar 2020).
- N. Trebesch* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *School of Molecular and Cellular Biology Retreat*. Champaign, IL (6 Sep 2019).
- N. Trebesch* 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)
- N. Trebesch* 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).
- N. Trebesch* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *Beckman Institute Graduate Student Seminar*. Urbana, IL (7 Nov 2018).
- N. Trebesch* 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).
- N. Trebesch* 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)
- N. Trebesch* and E. Tajkhorshid. "Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures." *Biophysical Society 62nd Annual Meeting*. San Francisco, CA (21 Feb 2018).
- N. Trebesch* 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).
- N. Trebesch*. "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)

- N. Trebesch*. "Atomistic Modeling and Simulation of Cell-Scale Membrane Structures with xMAS Builder." *NAMD Developer Workshop*. Chicago, IL (22 May 2017).
- N. Trebesch*[†] 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, N. Trebesch, 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).
- N. Trebesch*. "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)*

- N. Trebesch* and E. Tajkhorshid. "Capturing the Structural Dynamics and Energetics of the Large-Scale Elevator Transition of NaCT." *Biophysical Society 69th Annual Meeting*. Los Angeles, CA (19 Feb 2025).
- N. Trebesch* and E. Tajkhorshid. "Revealing the Unresolved Binding Sites and Outward-Facing State of NaCT."
  - *Gordon Research Conference (GRC) on Membrane Transport Proteins*. Newry, ME (24-25 Jul 2024).
  - *Gordon Research Seminar (GRS) on Membrane Transport Proteins*. Newry, ME (21 Jul 2024).
  - *Biophysical Society 68th Annual Meeting*. Philadelphia, PA (11 Feb 2024).
- N. Trebesch* 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).
- N. Trebesch* and E. Tajkhorshid. "The Homology of Elevator and Rocking Bundle Transporters." *Biophysical Society 67th Annual Meeting*. San Diego, CA (21 Feb 2023).
- N. Trebesch* 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).
- N. Trebesch* and E. Tajkhorhsid. "Structural Phylogenetics Suggest Evolutionary Relationships Exist Between Most Elevator Transporters." *Biophysical Society 66th Annual Meeting*. San Francisco, CA (21 Feb 2022).
- N. Trebesch* and E. Tajkhorshid. "Embracing Biological Complexity in Atomistic Simulations of Cellular Membranes." *Biophysical Society 64th Annual Meeting*. San Diego, CA (16 Feb 2020).
- N. Trebesch* 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).
  - *Biophysical Society 63rd Annual Meeting*. Baltimore, MD (4 Mar 2019).
- N. Trebesch* and E. Tajkhorshid. "Modeling and Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures with xMAS Builder."
  - *8th Annual oSTEM National Conference*. Houston, TX (17 Nov 2018).
  - *Illinois Biophysics Society Biophysics Graduate Research and Networking Symposium*. Urbana, IL (30 Oct 2018).
  - *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).
- N. Trebesch* and E. Tajkhorshid. "Modeling and Characterizing the Structural and Thermodynamic Aspects of the Elevator Transport Mechanism of VcINDY."
  - *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).
  - *Illinois Biophysics Society Biophysics Graduate Research and Networking Symposium*. Urbana, IL (23 Oct 2017).
  - *UIUC New Graduate Student Welcome Reception*. Urbana, IL (28 Aug 2017).
  - *Gordon Research Conference (GRC) on Mechanisms of Membrane Transport.* New London, NH (28-29 Jun 2017).
- N. Trebesch*, 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 (UHP) Thesis*. (2014). <https://github.com/noahtreb/rxn-sys-sim>.
- <u>N. Trebesch</u>. "Updates and Improvements to Hy3S." *Hy3S - Hybrid Stochastic Simulation for Supercomputers*. (2013). <http://sourceforge.net/projects/hysss/files/Hy3S%20Simulation%20Programs/v2.0.1/>.
- <u>N. Trebesch</u> and B. Freund. "Brownian Motion of Ellipsoidal Particles." *Methods of Experimental Physics Projects*. (2013). <https://sites.google.com/a/umn.edu/mxp/student-projects/2013-spring/s13brownianmotion>.
- J. W. Halley, A. Schofield, and B. Berntson. "Use of magnetite as anode for electrolysis of water." *Journal of Applied Physics*. **111**:124911 (2012). (<u>Acknowledgement</u>).

*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).