Timothy C. Moore

Department of Chemical Engineering ◇ University of Michigan
mtimc @ umich.edu

EDUCATION

Vanderbilt University, Nashville, TN *December 2017*
Ph.D., Chemical Engineering
Ph.D. Advisor: Clare McCabe

North Carolina State University, Raleigh, NC *May 2011*
B.S., Chemical Engineering
Magna Cum Laude

RESEARCH EXPERIENCE

University of Michigan January 2018–Present
Postdoctoral Fellow, Glotzer Lab *Ann Arbor, MI*

- Investigate the self-assembly and phase behavior of anisotropic colloids and nanoparticles
- Contribute to research and compute-time proposals
- Directly advise and mentor Ph.D. students
- Manage undergraduate research group members
- Proposed and validated a host–guest–mediated self-assembly scheme [Publication 13]
- Developed an unsupervised machine learning model to study self-assembly pathways [Publication 11]

Vanderbilt University January 2012–December 2017
Graduate Research Assistant, McCabe Lab *Nashville, TN*

- Conducted computational investigations into the structure and morphology of lipids in the human skin barrier using fully atomistic and coarse-grained molecular models
- Developed a novel method for deriving coarse-grained force fields [Publication 2]
- Developed accurate CG models of water and lipids to enable the study of lipid self-assembly [Publications 7, 4, and 3]
- Discovered a unique lipid packing mechanism that is responsible for the non-ideality of multicomponent gel-phase bilayers [Publication 3]
- Used a combination of high-performance CPU and GPU computing to perform molecular dynamics simulations of simplified skin models to identify composition-morphology-property relationships of the skin barrier
- Mentored five undergraduate summer researchers, including two NSF REU fellows

LORD Corporation May 2010–August 2010
Research Intern *Cary, NC*

- Funded by the NC Space Grant/LORD Corporation Summer Internship Program
- Developed novel thermal interface materials for electronics applications
- Characterized thermal, adhesive, and rheological properties of synthesized materials
- Presented research findings at division-wide annual meeting

North Carolina State University April 2009–September 2009
Undergraduate Researcher, Novak Lab (dept. of Chemistry) *Raleigh, NC*

- Synthesized and characterized polycarbodiimides for their unique optical properties, using a variety of techniques, including solution polymerization, Fourier transform infrared spectroscopy, ^{1}H, ^{13}C, and ^{15}N NMR, and polarimetry

SCHOLARSHIP

Publications

[†]equal contribution

23. Liu, T., Young, C.-M., **Moore, T. C.**, Glotzer, S. C., and Solomon, M. J. Defect structures in colloidal crystals and their effect on grating diffraction structural color. *ACS Applied Materials & Interfaces* **17** (2025), pp. 8171–8182

22. Craven, N. C., Singh, R., Quach, C. D., Gilmer, J. B., Crawford, B., Marin-Rimoldi, E., Smith, R., DeFever, R., Dyukov, M. S., Fothergill, J. W., Jones, C., **Moore, T. C.**, Butler, B. L., Anderson, J. A., Iacovella, C. R., Jankowski, E., Maginn, E. J., Potoff, J. J., Glotzer, S. C., Cummings, P. T., McCabe, C., and Siepmann, J. I. Achieving reproducibility and replicability of molecular dynamics and monte carlo simulations using the molecular simulation design framework (mosdef). *Journal of Chemical & Engineering Data* **70** (2025), pp. 2178–2199

21. Lu, F., Zhang, Y., Dwyer, T., Michelson, A., **Moore, T. C.**, Yan, H., Kisslinger, K., Zhang, H., Chen, X., Glotzer, S. C., and Gang, O. Octo-diamond crystal of nanoscale tetrahedra with interchanging chiral motifs. *Nature Materials* **24** (2025), pp. 785–793

20. Zhong, Yaxu[†], **Moore, T. C.**[†], Dwyer, Tobias[†], Butrum-Griffith, A., Allen, V. R., Chen, J., Wang, Y., Cheng, F., Glotzer, S. C., and Ye, X. Engineering and direct imaging of nanocube self-assembly pathways. *Nature Chemical Engineering* **1** (2024), pp. 532–541

19. Marino, E., LaCour, R. A., **Moore, T. C.**, van Dongen, S. W., Keller, A. W., An, D., Yang, S., Rosen, D. J., Gouget, G., Tsai, E. H., Kagan, C. R., Kodger, T. E., Glotzer, S. C., and Murray, C. B. Crystallization of binary nanocrystal superlattices and the relevance of short-range attraction. *Nature Synthesis* **3** (2024), pp. 111–122

18. Dwyer, T., **Moore, T. C.**, Anderson, J. A., and Glotzer, S. C. Tunable assembly of host–guest colloidal crystals. *Soft Matter* **19** (2023), pp. 7011–7019

17. **Moore, T. C.**, Rivera-Rivera, L. Y., and Glotzer, S. C. Inverse design of triblock janus spheres for self-assembly of complex structures in the crystallization slot via digital alchemy. *Soft Matter* **19** (2023), pp. 2726–2736

16. Shamaprasad, P., Frame, C. O., **Moore, T. C.**, Yang, A., Iacovella, C. R., Bouwstra, J. A., Bunge, A. L., and McCabe, C. Using molecular simulation to understand the skin barrier. *Progress in Lipid Research* **88** (2022), p. 101184

15. LaCour, R. A., **Moore, T. C.**, and Glotzer, S. C. Tuning stoichiometry to promote formation of binary colloidal superlattices. *Physical Review Letters* **128** (2022)

14. Shamaprasad, P., **Moore, T. C.**, Xia, D., Iacovella, C. R., Bunge, A. L., and McCabe, C. Multiscale simulation of ternary stratum corneum lipid mixtures: Effects of cholesterol composition. *Langmuir* **38** (2022), pp. 7496–7511

13. **Moore, T. C.**, Anderson, J. A., and Glotzer, S. C. Shape-driven entropic self-assembly of an open, reconfigurable, binary host–guest colloidal crystal. *Soft Matter* **17** (2021), pp. 2840–2848

12. Yang, A., **Moore, T. C.**, Iacovella, C. R., Thompson, M., Moore, D. J., and McCabe, C. Examining tail and headgroup effects on binary and ternary gel-phase lipid bilayer structure. *The Journal of Physical Chemistry B* **124** (2020), pp. 3043–3053

11. Adorf, C. S., **Moore, T. C.**, Melle, Y., and Glotzer, S. C. Analysis of self-assembly pathways with unsupervised machine learning algorithms. *The Journal of Physical Chemistry B* **124** (2020), pp. 69–78

10. **Moore, T. C.**, Yang, A. H., Ogungbesan, O., Hartkamp, R., Iacovella, C. R., Zhang, Q., and McCabe, C. Influence of single-stranded DNA coatings on the interaction between graphene nanoflakes and lipid bilayers. *The Journal of Physical Chemistry B* **123** (2019), pp. 7711–7721

9. **Moore, T. C.**, Hartkamp, R., Iacovella, C. R., Bunge, A. L., and McCabe, C. Effect of ceramide tail length on the structure of model stratum corneum lipid bilayers. *Biophysical Journal* **114** (2018), pp. 3113–3123

8. Hartkamp, R., **Moore, T. C.**, Iacovella, C. R., Thompson, M. A., Bulsara, P. A., Moore, D. J., and McCabe, C. Composition dependence of water permeation across multicomponent gel-phase bilayers. *The Journal of Physical Chemistry B* **122** (2018), pp. 3113–3123

7. **Moore, T. C.**, Iacovella, C. R., Leonhard, A. C., Bunge, A. L., and McCabe, C. Molecular dynamics simulations of stratum corneum lipid mixtures: a multiscale perspective. *Biochemical and Biophysical Research Communications* **498** (2017), pp. 313–318

6. Hartkamp, R., **Moore, T. C.**, Iacovella, C. R., Thompson, M. A., Bulsara, P. A., Moore, D. J., and McCabe, C. Investigating the structure of multicomponent gel-phase lipid bilayers. *Biophysical Journal* **111** (2016), pp. 813–823

5. Hartkamp, R., **Moore, T. C.**, Iacovella, C. R., Thompson, M. A., Bulsara, P. A., Moore, D. J., and McCabe, C. Structural properties of phospholipid-based bilayers with long-chain alcohol molecules in the gel phase. *The Journal of Physical Chemistry B* **120** (2016), pp. 12863–12871

4. **Moore, T. C.**, Iacovella, C. R., Hartkamp, R., Bunge, A. L., and McCabe, C. A coarse-grained model of stratum corneum lipids: free fatty acids and ceramide NS. *The Journal of Physical Chemistry B* **120** (2016), pp. 9944–9958

3. **Moore, T. C.**, Iacovella, C. R., and McCabe, C. Development of a coarse-grained water forcefield via multistate iterative Boltzmann inversion. In *Foundations of Molecular Modeling and Simulation*. Springer (2016), pp. 37–52

2. **Moore, T. C.**, Iacovella, C. R., and McCabe, C. Derivation of coarse-grained potentials via multistate iterative Boltzmann inversion. *The Journal of Chemical Physics* **140** (2014), p. 224104

1. Guo, S., **Moore, T. C.**, Iacovella, C. R., Strickland, L. A., and McCabe, C. Simulation study of the structure and phase behavior of ceramide bilayers and the role of lipid headgroup chemistry. *Journal of Chemical Theory and Computation* **9** (2013), pp. 5116–5126

Invited talks

8. "Anisotropy as a tool for materials discovery and design," Squishy Physics Seminar Series, Harvard University School of Engineering and Applied Sciences, Cambridge, MA, December 4, 2024.

7. "peakyFinders: a semi-automated tool for advanced defect analysis," DNA 30, Johns Hopkins University, Baltimore, MD, September 20, 2024.

6. "Exploiting anisotropy for materials discovery and design," Special Topics Seminar, North Carolina State University Department of Materials Science and Engineering, Raleigh, NC, July 24, 2023.

5. "The role of anisotropy in colloidal self-assembly," Klotsa Group, University of North Carolina Department of Applied Physical Sciences, Chapel Hill, NC, June 9, 2023.

4. "Digital alchemy for the inverse design of patchy particles," Statistical Thermodynamics & Molecular Simulations (STMS) Seminar Series, Virtual, February 17, 2023.

3. "Exploiting anisotropy for materials discovery and design," Oak Ridge National Laboratory Chemical Sciences Division and Materials Science and Technology Division Seminar Series, Oak Ridge, TN, June 8, 2022.

2. "Coarse-Graining Molecular Models for Biomolecular Self-Assembly," Seminar in the Laboratory of Computational Science and Modeling, Ècole polytechnique fédérale de Lausanne (EPFL), Lausanne, Switzerland, March 26, 2021.

1. "Understanding the Structural Arrangements of Stratum Corneum Lipids With Molecular Simulation," Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley, NH, August 13–17, 2017 (see Awards).

Contributed talks and posters

30. "Understanding colloidal crystallization through simulation: design and assembly of anisotropic particles," MRS Fall Meeting & Exhibit, Boston, MA, December 3, 2024.

29. "Stable inter-Martensitic colloidal crystals," AIChE Annual Meeting, San Diego, CA, October 30, 2024.

28. "Digital alchemy for the inverse design of patchy particles," Foundations of Molecular Modeling and Simulation, Snowbird, UT, July 28–August 1, 2024 (poster).

27. "Solvent-mediated reconfiguration of gold nanocube superlattices: a case study on challenges and opportunities in modeling anisotropic nanoscale building blocks," Midwest Thermodynamics and Statistical Mechanics Conference, Ann Arbor, MI, June 12, 2024.

26. "Understanding the mechanisms of crystallization and reconfiguration of anisotropic nanoparticle superlattices," APS March Meeting, Minneapolis, MN, March 7, 2024.

25. "Understanding the mechanisms of crystallization and reconfiguration of anisotropic nanoparticle superlattices," AIChE Annual Meeting, Orlando, FL, November 6, 2023.

24. "A Design Strategy for Open Colloidal Structures," 97th ACS Colloid and Surface Science Symposium, Raleigh, NC, June 6, 2023.

23. "Digital alchemy for the inverse design of patchy particles," APS March Meeting, Las Vegas, NV, March 7, 2023.

22. "Digital alchemy for the inverse design of patchy particles," AIChE Annual Meeting, Phoenix, AZ, November 14, 2022.

21. "A Design Strategy for Open Colloidal Structures," Foundations of Molecular Modeling and Simulation, Delevan, WI, July 18, 2022 (poster).

20. "Digital alchemy for the inverse design of patchy particles," 96th ACS Colloid and Surface Science Symposium, Golden, CO, July 13, 2022.

19. "A Design Strategy for Open Colloidal Structures," APS March Meeting, Chicago, IL, March 17, 2022.

18. "Crystal-Phase Polymorphism in Nanoplates via Competition Between Energy and Entropy" AIChE Annual Meeting, Boston, MA, November 8, 2021.

17. "A Design Strategy for Open Colloidal Structures," AIChE Annual Meeting, Virtual, November 17, 2020.

16. "An Open Software Approach for Reproducible Research for Materials Design," Michigan Institute for Data Science Research Reproducibility Showcase, July 28, 2020.

15. "Influence of DNA Coating on the Interaction Between Graphene Nanoflakes and Lipid Bilayers," Foundations of Molecular Modeling and Simulation, Delevan, WI, July 15–20, 2018 (poster).

14. "Self-Assembly Simulations of Stratum Corneum Lipid Mixtures," AIChE Annual Meeting, Minneapolis, MN, October 29–November 3, 2017.

13. "The Effects of Composition and Ceramide Chain Length on Stratum Corneum Lipid Bilayer Structure," Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley, NH, August 13–17, 2017. (poster)

12. "Self-Assembly of Model Stratum Corneum Lipid Mixtures," Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley, NH, August 13–17, 2017 (poster).

11. "Development and Self-Assembly of Coarse-Grained Skin Lipid Models Derived via Multistate Iterative Boltzmann Inversion," AIChE Annual Meeting, San Francisco, CA, November 13–18, 2016.

10. "Development of Transferable Coarse-Grained Force Fields via Multistate Iterative Boltzmann Inversion," AIChE Annual Meeting, San Francisco, CA, November 13–18, 2016 (poster).

9. "Understanding the Structural Arrangements of Stratum Corneum Lipids Through Coarse-grained and Fully Atomistic Molecular Dynamics Simulations," Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley, NH, August 16–21, 2015 (poster).

8. "Self-Assembly Studies of Coarse-Grained Skin Lipids," Foundations of Molecular Modeling and Simulation, Mt. Hood, OR, July 12–16, 2015 (poster).

7. "Derivation of Coarse-Grained Lipid Potentials Using Multi-State Iterative Boltzmann Inversion," AIChE Annual Meeting, Atlanta, GA, November 18, 2014.

6. "Simulation Studies of the Structural and Thermotropic Phase Behavior of Pure Ceramide Bilayers," 15th Annual Nanoscience & Nanotechnology Forum, Vanderbilt University, November 12, 2014 (poster).

5. "Derivation of Coarse-Grained Lipid Potentials Using Multi-State Iterative Boltzmann Inversion," Southeast Regional Meeting of the American Chemical Society, Nashville, TN, October 16, 2014.

4. "Simulation Studies of the Structural and Thermotropic Phase Behavior of Pure Ceramide Bilayers," Biomolecular Structure, Dynamics, and Function: Membrane Proteins conference, Nashville, TN, May 2–3, 2014 (poster).

3. "Derivation of Coarse-grained Potentials Using Multi-state Iterative Boltzmann Inversion," Aachen Conference on Computational Engineering Science, Aachen, Germany, September 10, 2013 (poster).

2. "Simulation Studies of the Structural and Thermotropic Phase Behavior of Pure Ceramide Bilayers," Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley, NH, August 18–23, 2013 (poster).

1. "A Simulation Study of the Self-Assembly of Coarse-Grained Skin Lipids" CCP5 Summer School 2013: Methods in Molecular Simulations, Cardiff University, Cardiff, Wales, 2012 (poster).

Mentees

- Jen Bradley (2022–present): University of Michigan M.S. student
- Chih-Mei Young (2022–present): University of Michigan Ph.D. student
- Alex Lee (2021–present): University of Michigan Ph.D. student
- Luis Rivera-Rivera (2020–2022): University of Michigan Ph.D. student

- Tobias Dwyer (2020–present): University of Michigan Ph.D. student
- Peter Schwendeman (2020–present): Huron High School student
- Allen LaCour (2019–2022): University of Michigan Ph.D. student
- Dan Evans (2019–2021): University of Michigan Undergraduate Student
- Bradley Dice (2019–2021): University of Michigan Ph.D. student
- Simon Adorf (2018–2019): University of Michigan Ph.D. student
- Alex Yang (2016–2017): Vanderbilt University Ph.D. student
- Davy Yue (Summer 2016): Vanderbilt University undergraduate student
- Donna Xia (Summer 2016): VINSE REU fellow
- Anne Leonhard (Summer 2015): VINSE REU fellow
- Monica Sowers (Summer 2014): Vanderbilt University undergraduate student
- Phil Schapiro (Summer 2013): Vanderbilt University undergraduate student

Awards

- "Generalizable Tools" Category Winner at the 2020 Reproducibility Challenge hosted by the Michigan Institute for Data Science
- Selected to give oral presentation by judges at poster session of 2017 Gordon Research Conference on Barrier Function of Mammalian Skin
- Travel Award for Outstanding Contribution; one of 8 selections out of 57 participants Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley, NH, August 16–21, 2015.
- 1st place in the poster competition for "Derivation of Coarse-grained Potentials Using Multi-state Iterative Boltzmann Inversion" at the Aachen Conference on Computational Engineering Science, Aachen, Germany, September 10, 2013.
- 2010 NC Space Grant recipient

TEACHING EXPERIENCE

University of Michigan January 2019–April 2019
Participant, Postdoctoral Short Course on Teaching and Learning *Ann Arbor, MI*

- 10-week course designed to prepare postdoctoral scholars to teach effectively as future faculty members
- Learn how to teach within a research-based framework that describes how students learn best in STEM disciplines
- Course activities included many short teaching experiences, preparation and delivery of a full lesson, and completion of a course syllabus

Vanderbilt University January 2012–May 2012
Teaching Assistant, Modeling and Simulation in Chemical Engineering *Nashville, TN*

- Held office hours to assist students in understanding and applying numerical methods used in chemical engineering, including the use of MATLAB
- Led review sessions before exams
- Graded exams and weekly homework assignments

Vanderbilt University August 2011–December 2011
Teaching Assistant, Chemical Process Principles *Nashville, TN*

- Led problem sessions to enhance the hands-on learning experience of the class
- Held office hours to help students understand and solve homework problems relating to fundamental chemical engineering principles
- Led review sessions before exams
- Graded exams and weekly homework assignments

SERVICE AND OUTREACH

Referee activity

- Scientific Reports (1)
- ACS Nano (3)
- Biophysical Journal (2)
- Journal of Chemical Physics (1)
- Journal of Physical Chemistry (2)
- Journal of Molecular Modeling (2)

Activity at Society Meetings

- Session chair, "Self- and Directed Assembly," ACS Colloid and Surface Science Symposium, Raleigh, NC, June 5, 2023.

Chemical Engineering Graduate Student Symposium September 23, 2021
University of Michigan *Ann Arbor, MI*

- Judged poster and oral presentations by Ph.D. students in the Department of Chemical Engineering at the University of Michigan

Macromolecular Science and Engineering Symposium October 2018, October 2019
University of Michigan *Ann Arbor, MI*

- Evaluated the research and presentation skills of graduate students from across the Midwest region
- Provided in-person feedback to presenters on their presentation style

Engineering Graduate Symposium October 26, 2018
University of Michigan *Ann Arbor, MI*

- Judged posters and presentations for a special session for outstanding Ph.D. students

Metro Nashville Public Schools Science Days June 6, 2017

- 1 day filled with science-related activities for 5^{th} grade students
- Led demonstrations and hands-on activities illustrating observable molecular phenomena, including the temperature-dependence of the diffusion of food coloring in water, the effect of solution composition on buoyancy, and basic surfactant properties
- Answered student questions related to "what is it like being a scientist?"

Vanderbilt Molecular Modeling Cybercamp May 2017, May 2016, May 2014

- 1 day intensive course on molecular modeling methods
- Led introductory sessions on using Jupyter Notebooks and bash scripting
- Led mini-sessions on lipid surfactant self-assembly, giving overview of surfactants and assisting participants in running generic surfactant self-assembly simulations and visualization and analysis of results
- Assisted the participants during hands-on sessions

MoSDeF Hackathon February 16–17, 2017
Vanderbilt University *Nashville, TN*

- Workshop designed to introduce users to molecular simulation tools being developed in the McCabe and Cummings groups at Vanderbilt
- Assisted with setting up tutorials and answering questions during hands-on workshop

Vanderbilt Summer Academy June 2016, July 2015, July 2014, and July 2013
Vanderbilt University *Nashville, TN*

- Summer program to allow highly gifted rising 8^{th} graders the opportunity to learn about the research environment at Vanderbilt University
- Led a session describing what molecular modeling and simulation is and how it is a complement to theoretical and experimental techniques
- Perform hands-on demonstrations of several scientific and engineering concepts, including physical measurement, prediction using physical models, and observation of phase separation, diffusion, and tribological phenomena
- Answer questions participants have regarding college and getting involved with research

Governor's School for Emerging Technologies June 16, 2016
Vanderbilt University *Nashville, TN*

- Summer enrichment program for gifted rising high school juniors and seniors, designed to stimulate interest in STEM fields
- Led two interactive sessions introducing students to molecular dynamics techniques
- Introduce the scientific method by having students develop a hypothesis, test their hypothesis with simulation, and provide a physical explanation for trends in the data

Vanderbilt Students Volunteering for Science Fall 2013, Fall 2011

- Service organization at Vanderbilt University designed to bring inquiry-based, hands-on science lessons to local elementary and middle school students
- Designed and tested science lessons aimed at 5^{th} and 6^{th} grade students
- Travel to local schools with a four-member team and give hands-on lessons on basic scientific principles to build interest in science and engineering
- Answer student questions regarding the college preparation process