Rose K. Cersonsky

Education

2014–2019 **Ph.D.**, *University of Michigan*, Ann Arbor, MI.

Macromolecular Science and Engineering GPA: 3.74/4.0

Thesis: "Designing Particle Shapes for Self-Assembly of Novel Colloidal Crystals"

Thesis Advisor: Prof. Sharon Glotzer

2010–2014 **B.S. in Engineering**, *University of Connecticut*, Storrs, CT.

Materials Science and Engineering GPA: 3.86/4.0

Minor Concentration: Computer Science and Engineering

Magna Cum Laude, Honors Degree

Honors Thesis Advisor: Prof. Mu-Ping Nieh

Senior Thesis Advisors: Prof. Serge Nakhmanson, Dr. Hillary Huttenhower

Professional Experience

2019-present Postdoctoral Researcher with Prof. Michele Ceriotti.

Ecolè Polytechnique Fèdèrale de Lausanne, Lausanne, Switzerland.

Developed machine learning methods and software for analyzing atomistic simulations and datasets of materials and molecules

Investigated role of molecular geometry on hierarchical assemblies

2014–2019 Graduate Student Researcher with Prof. Sharon Glotzer,

University of Michigan, Ann Arbor, MI.

Investigated of the role of shape in free energy optimization of colloidal crystals and design of novel photonic materials

Contributed to open-source software packages for simulation and data management (HOOMD-blue and signac)

2014–2019 Freelance Tutor, WyzAnt, Inc., Ann Arbor, MI.

Mentored and tutored students in mathematics and computer programming, completing 300+ hours of instruction

2012, 2013 Intern, Structural Alloys (2012), Polymeric Materials (2013),

Pratt and Whitney, East Hartford, CT.

Developed surface treatments to promote adhesion, processing for polymer foams, and repair for coatings

Investigated effects of microstructural imperfections in jet engine alloys

2012-2014 Undergraduate Student Researcher with Prof. Mu-Ping Nieh,

SAFN Laboratory, Storrs, CT.

Investigated the effects of composition and preparation on film fluorescence

Societies and Affiliations

American Institute of Chemical Engineers (AIChE), Materials Research Society (MRS), American Chemical Society (ACS), American Physical Society (APS), Alpha Sigma Mu

Publications

Refereed Journal Articles

- 1. Cersonsky, Rose K, Helfrecht, B. A., Engel, E. A., Kliavinek, S. & Ceriotti, M. Improving Sample and Feature Selection with Principal Covariates Regression. Machine Learning: Science and Technology 2, 035038 (2021).
- 2. Cersonsky, Rose K., Antonaglia, J. A., Dice, B. D. & Glotzer, S. C. The Diversity of Three-Dimensional Photonic Crystals. *Nature Communications* **12**, 2543 (2021).
- 3. Helfrecht, B. A., Cersonsky, Rose K, Fraux, G. & Ceriotti, M. Structure-property maps with kernel principal covariates regression. Machine Learning: Science and Technology **1**, 045021 (2020).
- 4. Travitz, A., Muniz, A., Beckwith, J. K. & Cersonsky, Rose K. Bringing Science Education and Research together to REACT. American Soc. for Engineering Ed. doi:10. 18260/1-2--35030 (2020).
- 5. Fraux, G., Cersonsky, Rose K & Ceriotti, M. Chemiscope: Interactive structureproperty explorer for materials and molecules. J. Open Source Software 5, 2117 (2020).
- 6. Cersonsky, Rose K, Dshemuchadse, J., Antonaglia, J., van Anders, G. & Glotzer, S. C. Pressure-tunable photonic band gaps in an entropic colloidal crystal. Physical Review Materials 2, 125201 (2018).
- 7. Cersonsky, Rose K, van Anders, G., Dodd, P. M. & Glotzer, S. C. Relevance of packing to colloidal self-assembly. Proceedings of the National Academy of Sciences **115**, 1439–1444 (2018).
- 8. Cersonsky, Rose K, Foster, L. L., Ahn, T., Hall, R. J., Van Der Laan, H. L. & Scott, T. F. Augmenting Primary and Secondary Education with Polymer Science and Engineering. J. of Chemical Education 94, 1639–1646 (2017).

Monographs and Technical Reports

- 9. **Cersonsky, Rose K**. Designing Nanoparticles for Self-Assembly of Novel Materials (University of Michigan, 2019). https://deepblue.lib.umich.edu/handle/2027.42/ 153520>.
- 10. Cersonsky, Rose K. Design Rules for Composites from Resin Transfer Molded Polyimides. (Technical Report, University of Connecticut and Pratt & Whitney, 2014).
- Cersonsky, Rose K, Jang, H.-s. & Nieh, M.-P. Optimizing Polymer Fluorescence for Explosives Detection (University of Connecticut, 2014). https://opencommons.uconn. edu/srhonors_theses/388>.

In Preparation

- Cersonsky, Rose K, Fraux, G., Kliavinek, S., Goscinski, A., Helfrecht, B. A. & Ceriotti, M. scikit-COSMO: A Toolbox of Machine Learning Methods for Materials Science
- Cersonsky, Rose K., Pahknova, M., Engel, E. A. & Ceriotti, M. Identifying highstability motifs in molecular crystals
- 14. Gazzarini, E., Bercx, M., Cersonsky, Rose K, Adorf, C. S. & Marzari, N. The magic rule of 4: tackling emerging features in inorganic databases
- Zhou, Y., Cersonsky, Rose K & Glotzer, S. C. A New Route to the Diamond Colloidal Crystal

16. **Cersonsky, Rose K.** & De, S. in *Quantum Chemistry in the Age of Machine Learning* (ed Dral, P.) Chapter 6: Unsupervised Learning (Elsevier, 2022).

Honors and Awards

Honors

- Jun. 2021 Victor K. LaMer Award, ACS Colloids Division.
- Feb. 2019 Biointerfaces Institute Innovator Award, University of Michigan (UM).
- Oct. 2018 **Towner Award for Graduate Research**, *UM*, Honorable Mention.
- Oct. 2018 Charles G. Overberger Award for Excellence in Research, UM.
- Jan. 2018 North Campus Martin Luther King Spirit Award, UM.
- Oct. 2017 Nonna Hamilton Student Service Award, UM.
- 2016, 2017 Prof. Albert and Mrs. Yee Student Leadership Award, UM.
- April 2017 Chapter of the Year, ACS POLY/PMSE.
- May 2014 **Commencement Speaker**, *UConn*.
- May 2014 Outstanding Academic Achievement Award, School of Engineering, UConn.
- 2012-2014 **New England Scholar**, *UConn*.
 - 2011 Babbidge Scholar, UConn.
- 2010-2014 **Dean's List**, *UConn*.

Grants, Fellowships, and Scholarships

- 2018-2019 Rackham Predoctoral Fellowship, UM.
 - 2017 Science Communication Fellow, Museum of Natural History, UM.
- 2014-2018 Rackham Merit Fellowship, UM.
 - 2014 Michigan Institute for Computational Discovery and Engineering Fellowship, UM.
- 2013-2014 **GE Advanced Materials Endowment Scholarship**, *UConn*.
 - 2013 Marshall Scholarship Finalist.
 - 2013 Rhodes Scholarship Nominee.
- 2012-2013 Art McEvily Academic Scholarship, UConn.
- 2010-2014 Academic Excellence Scholarship, UConn.

Travel Awards

- Jul. 2018 National Science Foundation FOMMS Travel Award, National Science Foundation.
- Jan. 2018 Ovshinsky Student Travel Award, Americal Physical Society.
- Jan. 2018 DCOMP Travel Award, Americal Physical Society.

Presentation Awards

- Dec. 2019 Poster Award, Materials Research Society.
- Apr. 2017 **2nd Place, Student Presentations**, Materials Research Society.
- Nov. 2016 3rd Place, Student Posters, Engineering Graduate Symposium.
- Apr. 2016 **3rd Place, Student Posters**, *MICDE Symposium*.
- Oct. 2015 1st Place, Student Presentations, Macromolecular Science and Engineering Symposium.

Seminar and Conference Presentations

Seminars and Distinguished Lectures

- Virtual Seminar Virtual (US Army DEVCOM Soldier Center, Aug. 2021).
- Victor K. LaMer Dissertation Award Lecture Virtual (ACS Colloids, June 2021).
- 3. Biointerfaces Innovator Award Lecture University of Michigan, Ann Arbor, MI (Biointerfaces Institute, Apr. 2019).
- 4. Seminar Oxford University, Oxford, Great Britain (Oct. 2018).
- 5. Visiting Researcher Presentation Eidgenoessische Technische Hochschule (ETH), Zurich, Switzerland (Sept. 2018).
- Seminar Ecole Polytechnique Lausanne (EPFL), Lausanne, Switzerland (Sept. 2018).

National Meetings, Workshops, and Conferences

- 7. APS March Meeting Virtual. Oral Presentation (Mar. 2021).
- MRS Fall Meeting Boston, MA. Poster, Poster Award for Session (Dec. 2019).
- 9. AIChE Annual Meeting Orlando, FL. Oral Presentation (Oct. 2019).
- 10. APS March Meeting Boston, MA. Oral Presentation (Mar. 2019).
- 11. MRS Fall Meeting Boston, MA. Oral Presentation (Nov. 2018).
- AIChE Annual Meeting Pittsburgh, PA. Oral Presentation (Oct. 2018).
- 13. Anisotropic Particles Symposium Konstanz, Germany. Oral Presentation (Sept. 2018).
- 14. Self-Assembly of Colloidal Systems Bordeaux, France. Oral Presentation (Sept. 2018).
- 15. Foundations of Molecular Modeling and Simulation Delavan, WI. Poster (July 2018).
- 16. APS March Meeting Los Angeles, CA. Oral Presentation (Mar. 2018).
- 17. AIChE Annual Meeting Minneapolis, MN. Oral Presentation (Nov. 2017).
- 18. Macromolecular Science and Engineering Symposium University of Michigan, Ann Arbor, MI. Poster (Oct. 2017).
- MRS Meeting Phoenix, AZ. Oral Presentation, 2nd Place for Presentations (Apr. 2017). 19.
- ACS Meeting San Francisco, CA. Oral Presentation (Apr. 2017). 20.
- 21. APS March Meeting New Orleans, LA. Oral Presentation (Mar. 2017).
- Engineering Graduate Symposium University of Michigan, Ann Arbor, MI. Poster, 3rd 22. Place for Posters (Nov. 2016).
- Macromolecular Science and Engineering Symposium University of Michigan, Ann Arbor, 23. MI. Poster (Oct. 2016).
- Michigan Institute for Computational Discovery and Engineering Symposium University of Michigan, Ann Arbor, MI. Poster, 3rd Place for Posters (Apr. 2016).
- Macromolecular Science and Engineering Symposium University of Michigan, Ann Arbor, 25. MI. Poster, 1st Place for Posters (Oct. 2015).
- Soft Matter Summer School University of Massachusetts, Amherst, MA. Poster (June 26. 2015).
- Senior Design Exposition UConn, Storrs, CT. Poster (May 2014). 27.

Workshops and Events Organized

- Oct. 2018 **Student Coordinator**, *Macromolecular Science and Engineering Symposium*.
- 2017-2019 Creator, Lead Organizer, Research Education and Activities for Classroom Teachers (REACT).

Developed and lead workshop for Michigan K-12 STEM teachers on UM campus, including coached student talks, lab tours, and demonstrations of hands-on activities by student organizations, and coordinating support from 10+ university departments and 20+ professors.

- June 2016 Organizer, The Life and Death of Plastics, UM XPlore Engineering.
- Sept. 2013 Head Curator, Master of Ceremonies, TEDxUConn 2013: "Future in Focus".

Workshop Participation

- Jun. 2021 Local Structure meets Machine Learning in Soft Matter, Centre Européen de Calcul Atomique et Moléculaire (CECAM).
- Sept. 2019 Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM, CECAM.
- Sept. 2018 Self-Assembly of Colloidal Systems, Université de Bordeaux.
- Oct. 2017 Science Communication Fellows Workshop, University of Michigan Natural History Museum.
- Sept. 2015 **Soft Matter Summer School**, *University of Massachusetts at Amherst*.

Teaching Experience and Service

Mentorship and Supervision of Junior Researchers

- 2020-present **Sergei Kliavinek**, Semester Project Student, EPFL.
 - Project: Comparing Feature Spaces for Materials and Molecules. Publication in Machine Learning, Science and Technology [1]
 - 2020-2021 Maria Pakhnova, Project Inspire Student, EPFL. Project: Identifying High-Stability Components of Molecular Crystals. Publication in preparation.
 - 2020-2021 **Pengkang Guo**, Semester Project Student, EPFL. Project: Implementing Dimensionality Reduction with Kernel PCovR Analysis.
 - 2019-2021 Benjamin Helfrecht, PhD Student, EPFL. Project Name: Structure-property maps with kernel principal covariates regression, Publication in Machine Learning, Science and Technology [3]
 - 2018-2020 **Yuan Zhou**, PhD Student, University of Michigan. Project: A new possibility for making diamond colloidal crystals. Publication in preparation [15].
 - 2016-2018 Alyssa Travitz, PhD Student, University of Michigan. Mentored through University of Michigan Mentorship Program, Publication in ASEE proceedings [4].
 - 2017-2018 **Sophie Barterian**, *Undergraduate Student*, *University of Michigan*. Project: When don't Colloids form FCC? Presented by Barterian at 2018 APS March Meeting

Service and Leadership

2017 **Student Ally**, UM Diversity, Equity, and Inclusion Strategic Plan.

2015-2019 Outreach Chair, UM ACS POLY/PMSE Student Chapter.

2010-2014 **Vice President**, *UTC UConn Engineering Ambassadors*.

2013-2014 **Vice President, Curation**, *TEDxUConn*.

Professional Skills

Coding Proficiencies: Python (Advanced),

Java (Intermediate-Advanced). MATLAB (Intermediate),

LATEX, git, bash/UNIX scripting, Scheme,

Python packages: MatPlotLib, NumPy, SciPy, IPython/Jupyter

Languages: English (Native) German (Conversational)

Spanish (Conversational) French (Beginner)

Contributions to Open-Source Software

All contributions can be found on GitHub page: https://github.com/rosecers.

Lead Developer

- 1. Kernel-Tutorials. a set of tutorials introducing users to kernel-based machine learning *methods* <https://github.com/cosmo-epfl/kernel-tutorials>.
- 2. scikit-COSMO. a package of functions modeled after scikit-learn (sklearn) including machine learning tools, some of which have been extended for materials science and chemical physics https://github.com/cosmo-epfl/sklearn-cosmo>.

Core Developer

3. Chemiscope. a visualization suite for correlating mapped data with 3D molecular visualization https://github.com/cosmo-epfl/chemiscope/>.

Contributor

- 4. Freud. a simple, flexible, powerful set of tools for analyzing trajectories obtained from molecular dynamics or Monte Carlo simulations https://github.com/glotzerlab/ freud>.
- 5. Freud-Examples. a repository of examples to employ the Freud module https://github. com/glotzerlab/freud-examples>.
- 6. LibRascal. a versatile and scalable fingerprint and machine learning code. It focuses on the efficient construction of representations of atomic structures, that can then be fed to any supervised or unsupervised learning algorithm .
- 7. Plato. efficient visualization of particle data https://github.com/glotzerlab/plato.
- 8. Pythia. generate numerical descriptions of particle systems < https://github.com/ glotzerlab/pythia>.
- 9. Signac. provides a simple and robust data model to create a well-defined indexable storage layout for data and metadata. https://github.com/glotzerlab/signac.

Signac-Flow. provides the basic components to set up simple to complex workflows for projects as part of the signac framework, including the submission of operations to high-performance super computers https://github.com/glotzerlab/signac-flow.

Personal Interests

Running (Baltimore Marathon Finisher 2016), Baking, Hiking, Rock Climbing, Bridge, Backgammon, Calligraphy

Performing Arts

- 2017-2019 **Technical Vocal Study**, *Instructor: Rachel Barg.*
 - 2015 **Featured Actor**, Big Fish, The Croswell Opera House, Crosswell, MI.
 - 2014 Leading Role, Sherlock Holmes and the Case of the Jersey Lily, UConn Dramatic PAWS, Storrs, CT.
 - 2013 Leading Role, Original Cast, Never Alone, UConn Dramatic PAWS, Storrs,
 - 2013 Leading Role, Fiorello!, The Gary-The Olivia at the Abbey of Regina Laudis, Bethlehem, CT.
 - 2010 **Featured Actor**, South Pacific, The Gary-The Olivia at the Abbey of Regina Laudis, Bethlehem, CT.
 - 2009 **Featured Actor**, The Pajama Game, The Gary-The Olivia at the Abbey of Regina Laudis, Bethlehem, CT.
 - 2008 Featured Actor, West Side Story, The Gary-The Olivia at the Abbey of Regina Laudis, Bethlehem, CT.