Rose K. Cersonsky

EPFL STI IMX COSMO. MXG 340, Station 12, CH-1015 Lausanne, Switzerland

> ⋈ rose.cersonsky@epfl.ch RoseCersonsky.com rosecers

Education

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

Macromolecular Science and Engineering

Thesis: "Designing Nanoparticles for Self-Assembly of Novel Materials"

Thesis Advisor: Prof. Sharon C. Glotzer

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

Materials Science and Engineering

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

- 2023– Assistant Professor, Chemical and Biological Engineering, University of Wisconsin, Madison, Madison, WI.
- 2019–2022 Postdoctoral Researcher with Prof. Michele Ceriotti, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland. Developed machine learning methods and implemented software for analyzing atomistic simulations and datasets of materials and molecules Investigated role of molecular interactions in hierarchical assemblies
- 2014–2019 Graduate Student Researcher with Prof. Sharon C. Glotzer, University of Michigan (UM), Ann Arbor, MI. Investigated 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, chemistry, 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

Publications

Refereed Journal Articles

- 1. Zhou, Y., Cersonsky, Rose K. & Glotzer, S. C. A route to hierarchical assembly of colloidal diamond. *Soft Matter* 18, 304–311 (2022).
- 2. **Cersonsky, R. 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).
- 3. Cersonsky, R. K., Antonaglia, J. A., Dice, B. D. & Glotzer, S. C. The Diversity of Three-Dimensional Photonic Crystals. *Nature Communications* 12, 2543 (2021).
- 4. Helfrecht, B. A., **Cersonsky, R. K.**, Fraux, G. & Ceriotti, M. Structure-property maps with kernel principal covariates regression. *Machine Learning: Science and Technology* 1, 045021 (2020).
- 5. Travitz, A., Muniz, A., Beckwith, J. K. & Cersonsky, R. K. Bringing Science Education and Research together to REACT. *ASEE* (2020).
- 6. Fraux, G., **Cersonsky, R. K.** & Ceriotti, M. Chemiscope: Interactive structure-property explorer for materials and molecules. *J. Open Source Soft.* **5**, 2117 (2020).
- 7. **Cersonsky, R. 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).
- 8. Cersonsky, R. K., van Anders, G., Dodd, P. M. & Glotzer, S. C. Relevance of packing to colloidal self-assembly. *PNAS* 115, 1439–1444 (2018).
- 9. Cersonsky, R. 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

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

Manuscripts Under Review or In Press

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

In Preparation

- 14. **Cersonsky, R. K.**, Fraux, G., Kliavinek, S., Goscinski, A., Helfrecht, B. A. & Ceriotti, M. *scikit-COSMO: A Toolbox of ML Methods for Materials Science*
- 15. **Cersonsky, R. K.**, Pahknova, M., Engel, E. A. & Ceriotti, M. *Identifying high-stability motifs in molecular crystals*
- 16. Gazzarini, E., Bercx, M., **Cersonsky, R. K.**, Adorf, C. S. & Marzari, N. The magic rule of 4: tackling emerging features in inorganic databases

Honors and Awards

Honors

- Jun. 2021 Victor K. LaMer Award, ACS Colloids Division.
- Feb. 2019 Biointerfaces Institute Innovator Award, 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.
 - 2017 Diversity, Equity, and Inclusion Ally, 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.
- 2012-2013 Art McEvily Academic Scholarship, UConn.
- 2010-2014 Academic Excellence Scholarship, UConn.

Travel Awards

- Nov. 2021 Women in Chemical Engineering Travel Award, AIChE.
 - 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.

Seminars, Conferences, and Workshops

Distinguished Lectures

- Victor K. LaMer Dissertation Award Lecture Virtual (ACS Colloids, June 2021).
- Biointerfaces Innovator Award Lecture University of Michigan, Ann Arbor, MI (Biointerfaces Institute, Apr. 2019).

Seminars and Invited Lectures

- Marvel Phase 2 Closing Event (Apr. 2022).
- University of Cambridge, Lennard-Jones Centre (Mar. 2022). 4.
- 5. Marvel Junior Seminar (Mar. 2022).
- University of California, Irvine, Materials Science and Engineering (Mar. 2022). 6.
- University of Denver, Mechanical and Materials Engineering (Feb. 2022). 7.
- 8. Boston University, College of Engineering (Feb. 2022).
- Northwestern University, Materials Science and Engineering (Feb. 2022).
- University of Minnesota, Chemical Engineering and Materials Science (Feb. 2022). 10.
- 11. Univ. of California, Berkeley, Chemical and Biomolecular Engineering (Jan. 2022).
- 12. Johns Hopkins University Materials Science and Engineering (Jan. 2022).
- 13. University of Wisconsin Chemical and Biological Engineering (Jan. 2022).
- 14. University of Amsterdam [hosted by AM Lab] (Jan. 2022).
- 15. Queen's University [hosted by Prof. Greg van Anders] (Jan. 2022).
- 16. Statistical Thermodynamics and Molecular Simulations (STMS) (Nov. 2021).
- 17. University of Michigan [hosted by Prof. Sharon C. Glotzer] (Oct. 2021).
- 18. US Army DEVCOM Soldier Center, Virtual (Aug. 2021).
- 19. Oxford University, Oxford, Great Britain (Oct. 2018).
- 20. Eidgenoessische Technische Hochschule (ETH), Zurich, Switzerland (Sept. 2018).
- 21. EPFL, Lausanne, Switzerland (Sept. 2018).

Oral Conference Presentations

- 22. MRS Annual Meeting Boston, MA. Session BI02 (Dec. 2021).
- 23. MRS Annual Meeting Boston, MA. Session CH04 (Nov. 2021).
- 24. AIChE Annual Meeting Boston, MA. 35i (Nov. 2021).
- 25. AIChE Annual Meeting Boston, MA. 127b (Nov. 2021).
- 26. AIChE Annual Meeting Boston, MA. 203e (Nov. 2021).
- 27. APS March Meeting Virtual. A60.9 (Mar. 2021).
- 28. APS March Meeting Cancelled. P43.7 (Mar. 2020).
- 29. AIChE Annual Meeting Orlando, FL. 502a (Oct. 2019).
- AIChE Annual Meeting Orlando, FL. 455c, presented by S. C. Glotzer (Oct. 2019). 30.
- APS March Meeting Boston, MA. C50.7 (Mar. 2019). 31.

- 32. MRS Fall Meeting Boston, MA. Session BM03 (Nov. 2018).
- 33. AIChE Annual Meeting Pittsburgh, PA. 276c (Oct. 2018).
- 34. Anisotropic Particles Symposium Konstanz, Germany (Sept. 2018).
- 35. Self-Assembly of Colloidal Systems Bordeaux, France (Sept. 2018).
- 36. APS March Meeting Los Angeles, CA. H12.12 (Mar. 2018).
- 37. AIChE Annual Meeting Minneapolis, MN. 704f (Nov. 2017).
- MRS Meeting Phoenix, AZ. CM3.3.05/CM7.2.05, 2nd Place Prize (Apr. 2017). 38.
- 39. ACS Meeting San Francisco, CA (Apr. 2017).
- 40. APS March Meeting New Orleans, LA. C17.02 (Mar. 2017).

Poster Presentations

- MRS Fall Meeting Boston, MA. Poster in Session EL01, Poster Award (Dec. 2019).
- 42. Foundations of Molecular Modeling & Simulation Delayan, WI. Poster (July 2018).
- 43. Macromolecular Science and Engineering Symposium University of Michigan, Ann Arbor, MI. Poster (Oct. 2017).
- 44. Engineering Graduate Symposium University of Michigan, Ann Arbor, MI. Poster, 3rd Place Prize (Nov. 2016).
- Macromolecular Science and Engineering Symposium University of Michigan, Ann 45.Arbor, MI. Poster (Oct. 2016).
- 46. Michigan Institute for Computational Discovery and Engineering Symposium University of Michigan, Ann Arbor, MI. Poster, 3rd Place Prize (Apr. 2016).
- 47. Macromolecular Science and Engineering Symposium University of Michigan, Ann Arbor, MI. Poster, 1st Place Prize (Oct. 2015).
- Soft Matter Summer School University of Massachusetts, Amherst, MA. Poster 48. (June 2015).
- Senior Design Exposition UConn, Storrs, CT. Poster (May 2014). 49.

Workshops and Events Organized

- Oct. 2018 Planning Committee, Macromolecular Sci. and Engr. 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 multiple university departments and professors.
- June 2016 Organizer, The Life and Death of Plastics, UM XPlore Engineering.
- Sept. 2013 Curator, Master of Ceremonies, TEDxUConn: "Future in Focus".

Workshop Participation

- Oct. 2021 MIT ChemE Rising Stars, Michigan Institute of Technology.
- Oct. 2021 NextProf Nexus, UM, Georgia Tech, University of California at Berkeley.

- 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 Workshop, UM Natural History Museum.
- Sept. 2015 Soft Matter Summer School, University of Massachusetts at Amherst.

Teaching Experience and Service

Mentorship and Supervision of Junior Researchers

- 2021-present Emma Lumiaro, Project Inspire Student, EPFL.
 - Project: Generalizing ML Potentials for Ensemble Learning of NMR Shieldings
- 2020-present Sergei Kliavinek, Semester Project Student, EPFL.
 - Project: Comparing Feature Spaces for Materials and Molecules. Publication in Machine Learning, Science and Technology [2]
 - 2020-2021 Maria Pakhnova, Project Inspire Student, EPFL.
 - Project: Identifying High-Stability Components of Molecular Crystals. Publica $tion\ in\ preparation.$
 - 2020-2021 **Pengkang Guo**, Semester Project Student, EPFL.
 - Project: Implementing Dimensionality Reduction with Kernel PCovR Analysis.
 - 2019-2021 Benjamin Helfrecht, PhD Student, EPFL.
 - Project: Structure-property maps with kernel principal covariates regression, Publication in Machine Learning, Science and Technology [4]
 - 2018-2020 Yuan Zhou, PhD Student, UM.
 - Project: A new possibility for making diamond colloidal crystals. Publication in Soft Matter/1].
 - 2016-2018 Alyssa Travitz, PhD Student, UM.
 - Mentored through UM Mentorship Program, Publication in ASEE [5].
 - 2017-2018 Sophie Barterian, Undergraduate Student, UM.
 - Project: When don't Colloids form FCC? Presented by SB at 2018 APS

Service and Leadership

- 2017 Student Ally, UM Diversity, Equity, and Inclusion Strategic Plan.
- 2017-2019 Creator and Lead Organizer, REACT.
- 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.
- 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/scikit-cosmo.

Core Developer

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-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 https://github.com/cosmoepfl/librascal.
- 7. Plato. efficient visualization of particle data https://github.com/glotzerlab/plato.
- 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 10. 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.
- 2013 2014 Leading Role, Original Cast, Various Productions, UConn Dramatic PAWS, Storrs, CT.
 - 2008-2013 Leading Role, Featured Actor, West Side Story, The Pajama Game, South Pacific, Fiorello!, The Gary-The Olivia at the Abbey of Regina Laudis, Bethlehem, CT.