

Rose K. Cersonsky

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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

- 2019–present **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

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, 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).
2. **Cersonsky, R. 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, R. 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, R. K.** Bringing Science Education and Research together to REACT. *ASEE* (2020).
5. Fraux, G., **Cersonsky, R. K.** & Ceriotti, M. Chemiscope: Interactive structure-property explorer for materials and molecules. *J. Open Source Soft.* **5**, 2117 (2020).
6. **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).
7. **Cersonsky, R. K.**, van Anders, G., Dodd, P. M. & Glotzer, S. C. Relevance of packing to colloidal self-assembly. *PNAS* **115**, 1439–1444 (2018).
8. **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

9. **Cersonsky, R. K.** *Designing Nanoparticles for Self-Assembly of Novel Materials* (University of Michigan, 2019). <https://hdl.handle.net/2027.42/153520>.
10. **Cersonsky, R. K.** *Design Rules for Composites from Resin Transfer Molded Polyimides*. (Tech. Report, University of Connecticut and Pratt & Whitney, 2014).
11. **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

12. Zhou, Y., **Cersonsky, R. K.** & Glotzer, S. C. *A Route to Hierarchical Assembly of Colloidal Diamond* <https://arxiv.org/abs/2111.04817v1>.
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

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

Seminars

3. Statistical Thermodynamics and Molecular Simulations (STMS) (Nov. 2021).
4. University of Michigan, Ann Arbor, MI (Oct. 2021).
5. US Army DEVCOM Soldier Center, Virtual (Aug. 2021).
6. Oxford University, Oxford, Great Britain (Oct. 2018).
7. Eidgenoessische Technische Hochschule (ETH), Zurich, Switzerland (Sept. 2018).
8. EPFL, Lausanne, Switzerland (Sept. 2018).

Oral Conference Presentations

9. *MRS Annual Meeting* Boston, MA. Session BI02 (Dec. 2021).
10. *MRS Annual Meeting* Boston, MA. Session CH04 (Nov. 2021).
11. *AIChE Annual Meeting* Boston, MA. 35i (Nov. 2021).
12. *AIChE Annual Meeting* Boston, MA. 127b (Nov. 2021).
13. *AIChE Annual Meeting* Boston, MA. 203e (Nov. 2021).
14. *APS March Meeting* Virtual. A60.9 (Mar. 2021).
15. *APS March Meeting* Cancelled. P43.7 (Mar. 2020).
16. *AIChE Annual Meeting* Orlando, FL. 502a (Oct. 2019).
17. *AIChE Annual Meeting* Orlando, FL. 455c, *presented by S. C. Glotzer* (Oct. 2019).
18. *APS March Meeting* Boston, MA. C50.7 (Mar. 2019).
19. *MRS Fall Meeting* Boston, MA. Session BM03 (Nov. 2018).
20. *AIChE Annual Meeting* Pittsburgh, PA. 276c (Oct. 2018).
21. *Anisotropic Particles Symposium* Konstanz, Germany (Sept. 2018).
22. *Self-Assembly of Colloidal Systems* Bordeaux, France (Sept. 2018).
23. *APS March Meeting* Los Angeles, CA. H12.12 (Mar. 2018).
24. *AIChE Annual Meeting* Minneapolis, MN. 704f (Nov. 2017).
25. *MRS Meeting* Phoenix, AZ. CM3.3.05/CM7.2.05, *2nd Place Prize* (Apr. 2017).
26. *ACS Meeting* San Francisco, CA (Apr. 2017).
27. *APS March Meeting* New Orleans, LA. C17.02 (Mar. 2017).

Poster Presentations

28. *MRS Fall Meeting* Boston, MA. Poster in Session EL01, Poster Award (Dec. 2019).
29. *Foundations of Molecular Modeling & Simulation* Delavan, WI. Poster (July 2018).

30. *Macromolecular Science and Engineering Symposium* University of Michigan, Ann Arbor, MI. Poster (Oct. 2017).
31. *Engineering Graduate Symposium* University of Michigan, Ann Arbor, MI. Poster, *3rd Place Prize* (Nov. 2016).
32. *Macromolecular Science and Engineering Symposium* University of Michigan, Ann Arbor, MI. Poster (Oct. 2016).
33. *Michigan Institute for Computational Discovery and Engineering Symposium* University of Michigan, Ann Arbor, MI. Poster, *3rd Place Prize* (Apr. 2016).
34. *Macromolecular Science and Engineering Symposium* University of Michigan, Ann Arbor, MI. Poster, *1st Place Prize* (Oct. 2015).
35. *Soft Matter Summer School* University of Massachusetts, Amherst, MA. Poster (June 2015).
36. *Senior Design Exposition* UConn, Storrs, CT. Poster (May 2014).

Workshops and Events Organized

Oct. 2018 **Planning Committee**, *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 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 Chemical Shieldings

- 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, UM*.
Project: A new possibility for making diamond colloidal crystals. *Publication under review [12]*.
- 2016-2018 **Alyssa Travitz**, *PhD Student, UM*.
Mentored through UM Mentorship Program, *Publication in ASEE [4]*.
- 2017-2018 **Sophie Barterian**, *Undergraduate Student, UM*.
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*.
- 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),
L^AT_EX, 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/scikit-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* <https://github.com/cosmo-epfl/librascal>.
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>.
10. *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 Crosswell 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, CT.
- 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.