

Rose K. Cersonsky

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📱 [rosecers](https://www.linkedin.com/in/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 (CBE)**,
University of Wisconsin, Madison (UW), Madison, WI.
- 2019–2022 **Postdoctoral Researcher with Prof. Michele Ceriotti**,
École Polytechnique Fédérale de Lausanne (EPFL), 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 colloidal crystals and the design of novel photonic materials
- 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.
- 2012–2014 **Undergraduate Student Researcher with Prof. Mu-Ping Nieh**,
SAFN Laboratory, Storrs, CT.

Publications

Peer-Reviewed Journal Articles

1. **Cersonsky, Rose K.**, Pakhnova, M., Engel, E. A. & Ceriotti, M. A data-driven interpretation of the stability of organic molecular crystals. *Chemical Science* (2023).
2. Zhou, Y., **Cersonsky, Rose K.** & Glotzer, S. C. A route to hierarchical assembly of colloidal diamond. *Soft Matter* **18**, 304–311 (2022).
3. **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).
4. **Cersonsky, R. K.**, Antonaglia, J. A., Dice, B. D. & Glotzer, S. C. The Diversity of Three-Dimensional Photonic Crystals. *Nature Communications* **12**, 2543 (2021).
5. 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).

6. Travitz, A., Muniz, A., Beckwith, J. K. & **Cersonsky, R. K.** Bringing Science Education and Research together to REACT. *ASEE* (2020).
7. Fraux, G., **Cersonsky, R. K.** & Ceriotti, M. Chemiscope: Interactive structure-property explorer for materials and molecules. *J. Open Source Soft.* **5**, 2117 (2020).
8. **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).
9. **Cersonsky, R. K.**, van Anders, G., Dodd, P. M. & Glotzer, S. C. Relevance of packing to colloidal self-assembly. *PNAS* **115**, 1439–1444 (2018).
10. **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).

In Press or Under Review

11. Cersonsky, T. E. K., **Cersonsky, R. K.**, Saade, G. R., Silver, R. M., Reddy, U. M., Goldenberg, R. L. & Pinar, H. Placental lesions associated with stillbirth by gestational age, according to feature importance: results from the Stillbirth Collaborative Research Network. In press at *Placenta*.
12. Pártay, L. B., Teich, E. G. & **Cersonsky, R. K.** Not Yet Defect-Free: The Current Landscape for Women in Computational Materials Research. In press at *npj Computational Materials*.

In Preparation

13. Lin, A., Huguenin-Dumittan Kevin K. nd Nigam, J., Crowley, A. C. & Nayak Saswat Kumar aand **Cersonsky, R. K.** Expanding Density-Correlation Machine Learning Formalisms for Anisotropic Particles.
14. Goscinski, A., Principe, V., Fraux, G., Kliavinek, S., Helfrecht, B. A., Ceriotti, M. & **Cersonsky, R. K.** scikit-matter: A Suite of Generalizable Machine Learning Methods Born out of Chemical and Materials Science.
15. Gazzarini, E., **Cersonsky, R. K.**, Bercx, M., Adorf, C. S. & Marzari, N. The magic rule of 4: tackling emerging features in inorganic databases.

Book Chapters

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

Monographs and Technical Reports

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

Open-Source Datasets

1. **Cersonsky, R. K.**, Pahknova, M., Engel, E. A. & Ceriotti, M. Lattice energies and relaxed geometries for 2'707 organic molecular crystals and their 3'242 molecular components. *Materials Cloud Archive* **5**. Interactive visualization at <http://molmotifs.matcloud.xyz>. <http://doi.org/10.24435/materialscloud:71-21> (2023).
2. Helfrecht, B. A., **Cersonsky, R. K.**, Fraux, G. & Ceriotti, M. Kernel principal covariates regression. *Materials Cloud Archive* **80**. <http://doi.org/10.24435/materialscloud:ay-eq> (2020).
3. **Cersonsky, R. K.**, Antonaglia, J. A., Dice, B. D. & Glotzer, S. *The Diversity of Three-Dimensional Photonic Crystals* 2021. <https://glotzerlab.engin.umich.edu/phonics/index.html>.

Honors and Awards

Honors

Jun. 2021 **Victor K. LaMer Award**, American Chemical Society (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**, *University of Connecticut (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 **MI 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

Jul. 2022 **National Science Foundation (NSF) FOMMS Travel Award**, *NSF*.
 Nov. 2021 **Women in Chemical Engineering Travel Award**, *American Institute of Chemical Engineers (AIChE)*.
 Jul. 2018 **NSF FOMMS Travel Award**, *NSF*.
 Jan. 2018 **Ovshinsky Student Travel Award**, *APS Division of Materials Physics (DMP)*.
 Jan. 2018 **Travel Award**, *APS Division of Computational Physics (DCOMP)*.

Presentation Awards

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

Seminars, Conferences, and Workshops

Distinguished Lectures

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

Seminars and Invited Lectures

3. *WCPM/HetSys Seminar* University of Warwick, Coventry, England (Oct. 2022).
4. *NRT-HDR: Harnessing AI for Design and Understanding Materials (aiM) Program* Duke University, Virtual (Sept. 2022).
5. *WiSFiRE: Women in STEM Frontiers in Research Expo* UConn, Virtual (Sept. 2022).
6. *Modeling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and Artificial Intelligence* Iris Adlershof Inst., Berlin, Germany. *Canceled due to illness* (July 2022).
7. *Marvel Phase 2 Closing Event* SwissTech Convention Center, Lausanne, Switzerland (Apr. 2022).
8. *Lennard-Jones Centre Seminar* University of Cambridge, Cambridge, England (Mar. 2022).
9. *Marvel Junior Seminar* NCCR Marvel, EPFL, Lausanne, Switzerland (Mar. 2022).

10. University of California, Irvine, Dept. of Materials Science and Engineering, Virtual (Mar. 2022).
11. University of Denver, Dept. of Mech. and Materials Engineering, Denver, CO (Feb. 2022).
12. Boston University, College of Engineering, Virtual (Feb. 2022).
13. Northwestern University, Materials Science and Engineering, Evanston, IL (Feb. 2022).
14. University of Minnesota, Chemical Eng. and Materials Science, Minneapolis, MN (Feb. 2022).
15. Univ. of California, Berkeley, Chemical and Biomolecular Engineering, Berkeley, CA (Jan. 2022).
16. Johns Hopkins University, Materials Science and Engineering, Baltimore, Maryland (Jan. 2022).
17. University of Wisconsin, Chemical and Biological Engineering, Virtual (Jan. 2022).
18. University of Amsterdam, AM Lab, Virtual (Jan. 2022).
19. Queen's University, Virtual (Jan. 2022).
20. Statistical Thermodynamics and Molecular Simulations (STMS), Virtual (Nov. 2021).
21. University of Michigan, Ann Arbor, MI (Oct. 2021).
22. US Army DEVCOM Soldier Center, Virtual (Aug. 2021).
23. Oxford University, Oxford, England (Oct. 2018).
24. Eidgenoessische Technische Hochschule (ETH), Zurich, Switzerland (Sept. 2018).
25. EPFL, Lausanne, Switzerland (Sept. 2018).

Oral Conference Presentations

26. *APS March Meeting* Las Vegas, NV. M28.9 (Mar. 2023).
27. *MRS Annual Meeting* Boston, MA. Session BI02 (Dec. 2021).
28. *MRS Annual Meeting* Boston, MA. Session CH04 (Nov. 2021).
29. *AIChE Annual Meeting* Boston, MA. 35i (Nov. 2021).
30. *AIChE Annual Meeting* Boston, MA. 127b (Nov. 2021).
31. *AIChE Annual Meeting* Boston, MA. 203e (Nov. 2021).
32. *APS March Meeting* Virtual. A60.9 (Mar. 2021).
33. *APS March Meeting* Cancelled. P43.7 (Mar. 2020).
34. *AIChE Annual Meeting* Orlando, FL. 502a (Oct. 2019).
35. *AIChE Annual Meeting* Orlando, FL. 455c, *presented by S. C. Glotzer* (Oct. 2019).
36. *APS March Meeting* Boston, MA. C50.7 (Mar. 2019).
37. *MRS Fall Meeting* Boston, MA. Session BM03 (Nov. 2018).
38. *AIChE Annual Meeting* Pittsburgh, PA. 276c (Oct. 2018).
39. *Anisotropic Particles Symposium* Konstanz, Germany (Sept. 2018).
40. *Self-Assembly of Colloidal Systems* Bordeaux, France (Sept. 2018).
41. *APS March Meeting* Los Angeles, CA. H12.12 (Mar. 2018).
42. *AIChE Annual Meeting* Minneapolis, MN. 704f (Nov. 2017).
43. *MRS Meeting* Phoenix, AZ. CM3.3.05/CM7.2.05, *2nd Place Prize* (Apr. 2017).
44. *ACS Meeting* San Francisco, CA (Apr. 2017).
45. *APS March Meeting* New Orleans, LA. C17.02 (Mar. 2017).

Poster Presentations

46. *Foundations of Molecular Modeling and Simulation* Delavan, WI (July 2022).
47. *MRS Fall Meeting* Boston, MA. Poster in Session EL01, Poster Award (Dec. 2019).
48. *Foundations of Molecular Modeling & Simulation* Delavan, WI. Poster (July 2018).
49. *Macromolecular Science and Engineering Symposium* UM, Ann Arbor, MI. Poster (Oct. 2017).
50. *Engineering Graduate Symposium* UM, Ann Arbor, MI. Poster, *3rd Place Prize* (Nov. 2016).
51. *Macromolecular Science and Engineering Symposium* UM, Ann Arbor, MI. Poster (Oct. 2016).

52. *Michigan Institute for Computational Discovery and Engineering Symposium* UM, Ann Arbor, MI. Poster, *3rd Place Prize* (Apr. 2016).
53. *Macromolecular Science and Engineering Symposium* UM, Ann Arbor, MI. Poster, *1st Place Prize* (Oct. 2015).
54. *Soft Matter Summer School* University of Massachusetts, Amherst, MA. Poster (June 2015).
55. *Senior Design Exposition* UConn, Storrs, CT. Poster (May 2014).

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

- 2023-present **Seungmin (Henry) Lee**, *Undergraduate Student, UW CBE*.
- 2023-present **Anna Claire Crowley**, *Undergraduate Student, UW CBE*.
- 2023-present **Natalie Hooven**, *Undergraduate Student, UW CBE*.
- 2022-present **Arthur Lin**, *PhD Student, UW CBE*.
- 2022-present **Saswat Nayak Kumar**, *PhD Student, UW CBE*.
- 2021-present **Victor Principe**, *PhD Student, EPFL IMX*, Approximating the Landscape of Molecular Crystals for NMR Shielding Predictions.
- 2020-2022 **Sergei Kliavinek**, *Semester Project Student, EPFL IMX*, Comparing Feature Spaces for Small Molecules. *Publication in MLST [3] and one forthcoming [14]*.
Current Position: PhD student at California Institute of Technology.
- 2021-2022 **Emma Lumiaro**, *Project Inspire Student, EPFL IMX*, Generalizing ML Potentials for Ensemble Learning of NMR Shieldings.
Current Position: Analytics Consultant at ESPOO
- 2020-2021 **Maria Pakhnova**, *Project Inspire Student, EPFL IMX*, Identifying High-Stability Components of Molecular Crystals. *Publication accepted to Chemical Science [1]*.
- 2020-2021 **Pengkang Guo**, *Semester Project Student, EPFL IMX*, Implementing Dimensionality Reduction with Kernel PCovR Analysis.
- 2019-2021 **Benjamin Helfrecht**, *PhD Student, EPFL IMX*, Structure-property maps with kernel principal covariates regression, *Publications in MLST [5], [3], and one forthcoming [14]*.
Current Position: Postdoctoral Researcher at Pacific Northwest National Laboratory

- 2018-2020 **Yuan Zhou**, *PhD Student, UM ChE*, A new possibility for making diamond colloidal crystals. *Publication in Soft Matter*[2].
- 2016-2018 **Alyssa Travitz**, *PhD Student, UM Macro*, Mentored through UM Mentorship Program, *Publication in ASEE* [6].
Current Position: RET Software Scientist at Intel
- 2017-2018 **Sophie Barterian**, *Undergraduate Student, UM Physics*, When don't Colloids form FCC? *Presented by SB at 2018 APS*.
Current Position: Assistant Audio Engineer at Iyuno-SDI Group

Service and Leadership

Peer Reviewer for: ACS Photonics, Nature Communications, Journal of Chemical Physics, Digital Discovery, AIP Advances, Soft Matter, Journal of Open Source Software

Guest Editor for: *Machine Learning of Thermophysical Properties* (Journal of Chemical Engineering Data, 2023)

- 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*.

Contributions to Open-Source Software

All contributions can be found on the Cersonsky lab GitHub page: <https://github.com/cersonsky-lab> and my personal 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/lab-cosmo/kernel-tutorials>.
2. *scikit-matter*. 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/lab-cosmo/scikit-matter>.
3. *AniSOAP*. A python package for computing the Density-Correlation Descriptors for Anisotropic Chemical Bodies <https://github.com/cersonsky-lab/anisoap/>.

Core Developer

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

Contributor

5. *Freud*. a simple, flexible, powerful set of tools for analyzing trajectories obtained from molecular dynamics or Monte Carlo simulations <https://github.com/glotzerlab/freud>.
6. *Freud-Examples*. a repository of examples to employ the *Freud* module <https://github.com/glotzerlab/freud-examples>.
7. *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/lab-cosmo/librascal>.
8. *Plato*. efficient visualization of particle data <https://github.com/glotzerlab/plato>.
9. *Pythia*. generate numerical descriptions of particle systems <https://github.com/glotzerlab/pythia>.
10. *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>.
11. *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>.

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)

Personal Interests

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

Performing Arts

Technical vocal study (Instructor: Rachel Barg) and musical theater performance: *Big Fish* (The Crosswell Opera House, Crosswell, MI), *West Side Story*, *The Pajama Game*, *South Pacific*, *Fiorello!* (The Gary-The Olivia at the Abbey of Regina Laudis, Bethlehem, CT), and various other productions.