Rose K. Cersonsky

⊠ rose.cersonsky@wisc.edu cersonsky-lab.github.io/website cersonsky-lab/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- Conway Assistant Professor, Chemical and Biological Engineering (CBE),

University of Wisconsin, Madison (UW), Madison, WI.

Data Science Affiliate Faculty

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.

Funds Raised

2023-2025 Wisconsin Research Forward Initiative, Wisconsin Alumni Research Foundation, Co-PI, \$32,267 personal funding across two years.

Collaboration with Profs. V. Zavala (CBE), R. van Lehn (CBE), M. Gebbie (CBE), J. Cisewski-Kehe

(Data Science), and F. Liu (MSE)

2023-2029 Wisconsin Materials Research Science and Engineering Center (MRSEC), National

Science Foundation, Co-PI, \$510,000 personal funding across six years.

Collaboration with Profs. M. Ediger (Chemistry), D. Morgan (MSE), J. Perepezko (MSE), I. Szlufarska (MSE), P. M. Voyles (MSE), B. Wang (CEE), L. Yu (Pharmacy) V. Zavala (CBE); Z. Fakhraai (Chemistry, U. Penn), Y. Su (Merck), G. Zhang (AbbVie), C. Benmore (ANL), L. Berthier (U. Montpellier)

Publications

Peer-Reviewed Journal Articles

1. Cersonsky, R. K., Pakhnova, M., Engel, E. A., Ceriotti, M., A data-driven interpretation of the stability of organic molecular crystals. Chemical Science 14, 1272–1285. ISSN: 2041-6520, 2041-6539. http://xlink.rsc.org/?DOI=D2SC06198H (Feb. 2023).

- Cersonsky, T. E. K. Cersonsky, R. K., Saade, G. R., Silver, R. M., Reddy, U. M., Goldenberg, R. L., Dudley, D. J., Pinar, H., Placental lesions associated with stillbirth by gestational age, according to feature importance: Results from the stillbirth collaborative research network. Placenta 137, 59-64. ISSN: 01434004. https://linkinghub.elsevier.com/retrieve/pii/S0143400423000760 (Apr. 2023).
- Goscinski, A., Principe, V. P., Fraux, G., Kliavinek, S., Helfrecht, B. A., Loche, P., Ceriotti, M., Cersonsky, R. K., scikit-matter: A Suite of Generalisable Machine Learning Methods Born out of Chemistry and Materials Science. Open Research Europe 3, 81. ISSN: 2732-5121. https://open-researcheurope.ec.europa.eu/articles/3-81/v1 (June 2023).
- 4. Pártay, L. B., Teich, E. G., Cersonsky, R. K., Not yet defect-free: the current landscape for women in computational materials research. npj Computational Materials 9, 98. ISSN: 2057-3960. https://www. nature.com/articles/s41524-023-01054-z (June 2023).
- Zhou, Y., Cersonsky, R. K., Glotzer, S. C., A route to hierarchical assembly of colloidal diamond. Soft Matter 18, 304–311. ISSN: 1744-683X, 1744-6848. http://xlink.rsc.org/?DOI=D1SM01418H (Jan. 2022).
- Cersonsky, R. K., Antonaglia, J., Dice, B. D., Glotzer, S. C., The diversity of three-dimensional photonic crystals. Nature Communications 12, 2543. ISSN: 2041-1723. https://www.nature.com/articles/s41467-021-22809-6 (May 2021).
- 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. ISSN: 2632-2153. https://iopscience.iop.org/article/10.1088/2632-2153/abfe7c (May 2021).
- Fraux, G., Cersonsky, R. K., Ceriotti, M., Chemiscope: interactive structure-property explorer for materials and molecules. Journal of Open Source Software 5, 2117. ISSN: 2475-9066. https://joss.theoj. org/papers/10.21105/joss.02117 (Nov. 2020).
- 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. ISSN: 2632-2153. https://iopscience.iop.org/article/10.1088/2632-2153/aba9ef (Oct. 2020).
- Travitz, A., Muniz, A., Beckwith, J., Cersonsky, R. K., Paper: Bringing Science Education and Research together to REACT in (ASEE Conferences, Virtual On line, June 2020), 35030. http://peer.asee.org/35030.
- 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. ISSN: 2475-9953. https://link.aps.org/doi/10.1103/PhysRevMaterials.2.125201 (Nov. 2018).
- Cersonsky, R. K., Van Anders, G., Dodd, P. M., Glotzer, S. C., Relevance of packing to colloidal selfassembly. Proceedings of the National Academy of Sciences 115, 1439–1444. ISSN: 0027-8424, 1091-6490. https://pnas.org/doi/full/10.1073/pnas.1720139115 (Feb. 2018).
- 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. Journal of Chemical Education 94, 1639–1646. ISSN: 0021-9584, 1938-1328. https://pubs.acs.org/doi/10.1021/acs.jchemed.6b00805 (Sept. 2017).

In Press or Under Review

- Allen, M., Bediako, K., Bowman, W., Calabrese, M., Caretta, L., Cersonsky, R. K., Chen, W., Correa, S., Davidson, R., Dresselhaus-Marais, L., Eisler, C. N., Furst, A., Ge, T., Hook, A., Hsu, Y.-T., Jia, C., Lu, J., Lunghi, A., Messina, M., Moreno-Hernandez, I. A., Nichols, E., Rao, R., Seifrid, M., Shulenberger, K. E., Simonov, A., Su, X., Swearer, D., Tang, E., Taylor, M., Tran, H., Trindade, G., Truby, R., Utzat, H., Yang, Y., Yee, D. W., Zhao, S., Cranford, S., 35+1 Challenges In Materials Science Being Tackled by PIs Under 35(ish) in 2023. *Matter* (July 2023).
- Cersonsky, T. E. K. Cersonsky, R. K., Silver, R. M., Dudley, D. J., Pinar, H., Placental lesions associated with stillbirth by gestational age, as related to cause of death: follow-up results from the Stillbirth Collaborative Research Network.

In Preparation

Gazzarini, E., Cersonsky, R. K., Bercx, M., Adorf, C. S., Marzari, N., The magic rule of 4: tackling emerging features in inorganic databases.

17. Lin, A., Huguenin-Dumittan, K. K., Nigam, J., Cersonsky, R. K., Expanding Density-Correlation Machine Learning Formalisms for Anisotropic Particles. *Preparation*.

Book Chapters

1. Cersonsky, R. K., De, S., in Quantum Chemistry in the Age of Machine Learning 153–181 (Elsevier, Jan. 2023). ISBN: 978-0-323-90049-2. https://linkinghub.elsevier.com/retrieve/pii/B9780323900492000251.

Monographs and Technical Reports

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

Open-Source Datasets

- 1. Cersonsky, R., Pakhnova, M., Engel, E., Ceriotti, M., Lattice energies and relaxed geometries for 2'707 organic molecular crystals and their 3'242 molecular components. Feb. 2023. https://archive. materialscloud.org/record/2023.5.
- 2. Cersonsky, R. K., Antonaglia, J. A., Dice, B. D., Glotzer, S., The Diversity of Three-Dimensional Photonic Crystals May 2021. https://glotzerlab.engin.umich.edu/photonics/index.html.
- Helfrecht, B. A., Cersonsky, R. K., Fraux, G., Ceriotti, M., Structure-property maps with kernel principal covariates regression Oct. 2020. https://archive.materialscloud.org/record/2020.80.

Honors and Awards

Honors

- Jul. 2023 **35 under 35**, *Matter*.
- 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

- Victor K. LaMer Award Distinguished Lecture ACS Colloids (June 2021).
- Biointerfaces Innovator Award Lecture UM (Biointerfaces Institute, Apr. 2019).

Seminars and Invited Lectures

- Invited Lecture Iowa State (July 2023).
- Invited Lecture University of Southhampton (May 2023).
- 5. Panel, Exploring AI at University of Wisconsin - Madison (June 2023).
- 6. Machine Learning and Chemistry: Are we there yet? University of Maryland, College Park (May 2023).
- 7. Harnessing AI for Design and Understanding Materials Program Duke University (Sept. 2022).
- 8. Marvel Phase 2 Closing Event SwissTech Convention Center (Apr. 2022).
- Marvel Junior Seminar NCCR Marvel, EPFL (Mar. 2022). 9.
- 10. Lennard-Jones Centre Seminar University of Cambridge, Cambridge, UK (Mar. 2022).
- Modeling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and Artificial 11. Intelligence Iris Adlershof Institute, Berlin, Germany (July 2022).
- 12. WiSFiRE: Women in STEM Frontiers in Research Expo UConn (Sept. 2022).
- Invited Lecture Queen's University (Jan. 2022).
- 14. Invited Seminar University of Wisconsin, Chemical and Biological Engineering (Jan. 2022).
- 15. Invited Seminar University of California, Irvine, Dept. of Materials Science and Engineering (Mar. 2022).
- 16. Invited Seminar Johns Hopkins University, Materials Science and Engineering (Jan. 2022).
- 17. Invited Seminar University of Minnesota, Chemical Eng. and Materials Science (Feb. 2022).
- 18. Invited Seminar University of Denver, Dept. of Mech. and Materials Engineering (Feb. 2022).
- 19. Invited Seminar Northwestern University, Materials Science and Engineering (Feb. 2022).
- 20. Invited Seminar University of California, Berkeley, Chemical and Biomolecular Engineering (Jan. 2022).
- 21. Invited Seminar Boston University, College of Engineering (Feb. 2022).
- 22. Invited Seminar University of Amsterdam, AM Lab (Jan. 2022).
- 23. WCPM/HetSys Seminar University of Warwick, Coventry, UK (Oct. 2022).
- 24. Hybrid Unsupervised-Supervised Machine Learning Models for Molecular Science Statistical Thermodynamics and Molecular Simulations (STMS) (Nov. 2021).
- 25. Invited Lecture University of Michigan (Oct. 2021).
- 26. Invited Seminar US Army DEVCOM Soldier Center (Aug. 2021).
- 27. Invited Seminar Oxford University (Oct. 2018).
- 28. Invited Seminar Eidgenoessische Technische Hochschule (ETH) (Sept. 2018).

29. Invited Seminar EPFL (Sept. 2018).

Oral Conference Presentations

- Leveraging Machine-Learning for the Structure-Property Paradigm ACS Colloids and Interfaces, University of North Carolina (June 2023).
- 31. A data-driven interpretation of the stability of molecular crystals APS March Meeting. M28.9 (Mar. 2023).
- 32. The Search for Novel Mesoscale Materials AIChE Annual Meeting. 127b (Nov. 2021).
- Enhanced Machine Learning Models for Structure-Property Mapping with Principal Covariates Regression APS March Meeting. A60.9 (Mar. 2021).
- 34. Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression MRS Annual Meeting. Session CH04 (Nov. 2021).
- Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression AIChE Annual 35. Meeting. 203e (Nov. 2021).
- The Diversity of Three-Dimensional Photonic Crystals for Colloidal Self-Assembly MRS Annual Meeting. 36. Session BI02 (Dec. 2021).
- 37. The Diversity of Three-Dimensional Photonic Crystals for Colloidal Self-Assembly AIChE Annual Meeting. 35i (Nov. 2021).
- 38. Unexpected Photonic Band Gaps in 3D Crystal Structures APS March Meeting, Cancelled. P43.7 (Mar. 2020).
- 39. A New Possibility for Making Diamond Colloidal Crys AIChE Annual Meeting. 183g, presented by Yuan Zhou (Nov. 2020).
- In Search of the Photonic Band Gap AIChE Annual Meeting. 455c, presented by S. C. Glotzer (Oct. 40.
- Understanding Photonic Band Gaps in Three Dimensions AIChE Annual Meeting. 502a (Oct. 2019). 41.
- Can we design a reconfigurable photonic crystal in the visible light range? APS March Meeting. C50.7 (Mar. 2019).
- 43. Pressure-Tunable Photonic Band Gaps in an Entropic Colloidal Crystal AIChE Annual Meeting. 276c (Oct. 2018).
- 44. Pressure-Tunable Photonic Band Gaps in an Entropic Colloidal Crystal MRS Fall Meeting. Session BM03 (Nov. 2018).
- Tunable Photonic Band Gaps in an Entropic Crystal APS March Meeting. H12.12 (Mar. 2018). 45.
- 46. Tunable Photonic Band Gaps in an Entropic Crystal Anisotropic Particles Symposium, Konstanz, Germany (Sept. 2018).
- Tunable Photonic Band Gaps in an Entropic Crystal Self-Assembly of Colloidal Systems, Bordeaux, France (Sept. 2018).
- Augmenting Primary and Secondary Education with Polymer Science and Engineering ACS Meeting 48. (Apr. 2017).
- 49. Insights into Inverse Materials Design from Phase Transitions in Shape Space MRS Meeting. CM3.3.05/CM7.2.05, 2^{nd} Place Prize (Apr. 2017).
- Insights into Inverse Materials Design from Phase Transitions in Shape Space AIChE Annual Meeting. 50. 704f (Nov. 2017).
- Insights into Inverse Materials Design from Phase Transitions in Shape Space APS March Meeting. C17.02 (Mar. 2017).

Poster Presentations

- 52. Foundations of Molecular Modeling and Simulation Delayan, WI (July 2022).
- MRS Fall Meeting Boston, MA. poster in Session EL01, poster Award (Dec. 2019). 53.
- 54. When don't colloids order into cubic-close packings? APS March Meeting. L60.144, presented by S. Barterian (Mar. 2018).

- Foundations of Molecular Modeling & Simulation Delayan, WI. poster (July 2018). 55.
- Macromolecular Science and Engineering Symposium UM, Ann Arbor, MI. poster (Oct. 2017). 56.
- Engineering Graduate Symposium. poster, 3rd Place Prize (Nov. 2016). 57.
- 58. Macromolecular Science and Engineering Symposium UM, Ann Arbor, MI. poster (Oct. 2016).
- Michigan Institute for Computational Discovery and Engineering Symposium UM, Ann Arbor, MI. poster, 3rd Place Prize (Apr. 2016).
- Soft Matter Summer School University of Massachusetts. poster (June 2015).
- Macromolecular Science and Engineering Symposium UM, Ann Arbor, MI. poster, 1st Place Prize (Oct. 2015).

Teaching and Mentorship

Courses Taught at UW-Madison

- Spring 2023 CBE 440, Chemical Engineering Materials.
 - Fall 2023 CBE 710, Advanced Chemical Engineering Thermodynamics.

Courses and Workshops outside UW-Madison

Jul. 2023 Unsupervised Learning, iCOMSE Workshop on Machine Learning for Molecular Simulation, Minneapolis, MN.

Mentorship and Supervision of Junior Researchers

Undergraduate Researchers

- 2023-present Yong-Cheol Cho, UW CBE and CSE.
- 2023-present Caleb Youngwerth, UW Chemistry.
- 2023-present Seungmin (Henry) Lee, UW CBE.
- 2023-present Anna Claire Crowley, UW CBE.
- 2023-present Natalie Hooven, UW CBE.

Graduate Researchers

- 2022-present Arthur Lin, UW CBE.
- 2022-present Saswat Kumar Nayak, UW CBE.

Advisees prior to 2023

- 2021-2023 Victor Principe, PhD Student, EPFL IMX, Approximating the Landscape of Molecular Crystals for NMR Shielding Predictions, Publications in ORE [3].
- 2020-2022 Sergei Kliavinek, Semester Project Student, EPFL IMX, Comparing Feature Spaces for Small Molecules. Publications in MLST [7] and ORE [3]. 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 in Chemical Science [1]. Incoming PhD student at UW-Madison
- 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 [3], [7], and ORE [3]. Current Position: Postdoctoral Reseacher 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/5].
 - Current Position: Data scientist with Huawei

- 2016-2018 Alyssa Travitz, PhD Student, UM Macro, Mentored through UM Mentorship Program, Publication in ASEE [10].
 - 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

Professional Service and Leadership

University of Wisconsin Committees: Diversity, Equity, and Inclusion (2023-present), Graduate Admissions (2023-present)

Peer Reviewer for: ACS Photonics, Nature Communications, Journal of Chemical Physics, Digital Discovery, AIP Advances, Soft Matter, Journal of Open Source Software, Journal of Physical Chemistry A, Journal of Chemical Theory and Computation, NSF Division of Electronics and Photonics

- Dec. 2023 Guest Editor, Machine Learning of Thermophysical Properties, Journal of Chemical and Engineering Data.
- 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.

- 2015-2019 Outreach Chair, UM ACS POLY/PMSE Student Chapter.
- Oct. 2018 Planning Committee, Macromolecular Sci. and Engr. Symposium.
 - 2017 Student Ally, UM Diversity, Equity, and Inclusion Strategic Plan.
- June 2016 Organizer, The Life and Death of Plastics, UM XPlore Engineering.
- 2010-2014 Vice President, UTC UConn Engineering Ambassadors.
- 2013-2014 Vice President, Curation, TEDxUConn.
- 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.

Software Proficiency and Development

All open-source 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. AniSOAP. A python package for computing the Density-Correlation Descriptors for Anisotropic Chemical Bodies https://github.com/cersonsky-lab/anisoap/.
- 2. Kernel-Tutorials. a set of tutorials introducing users to kernel-based machine learning methods https: //github.com/lab-cosmo/kernel-tutorials.
- 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- \cos mo/scikit-matter.

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.
- Freud-Examples. a repository of examples to employ the Freud module https://github.com/glotzerlab/ freud-examples.
- 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.
- Plato. efficient visualization of particle data https://github.com/glotzerlab/plato.
- Pythia. generate numerical descriptions of particle systems https://github.com/glotzerlab/pythia.
- 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.

Coding Proficiencies: Python (Native),

TypeScript, Java, MATLAB

LATEX, git, bash/UNIX scripting, Scheme,

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

This is not a comprehensive list.

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 Croswell 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.