Rose K. Cersonsky, Ph.D.

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Education

2014–2019 **Ph.D.**, *University of Michigan*, Ann Arbor, MI, USA, 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, USA, 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–present **Conway Assistant Professor, Chemical and Biological Engineering (CBE)**, University of Wisconsin, Madison (UW), Madison, WI, USA.
Affiliate of the Data Science Institute
Materials Science and Engineering 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 crystallization via first-principles methods

2014–2019 **Graduate Student Researcher with Prof. Sharon C. Glotzer**,
University of Michigan (UM), Ann Arbor, MI, USA.
Investigated the role of shape in colloidal assembly and the design of novel photonic materials

2012, 2013 **Intern, Structural Alloys (2012), Polymeric Materials (2013)**,
Pratt and Whitney, East Hartford, CT, USA.

2012-2014 **Undergraduate Student Researcher with Prof. Mu-Ping Nieh**,
Self-Assembly of Functional Nanomaterials (SAFN) Laboratory, Storrs, CT, USA.
Synthesized and characterized fluorescence of polymer files for explosives detection

Publications

Peer-Reviewed Journal Articles and Pre-prints

1. Jorgensen, C., Lin, A. Y. & Cersonsky, R. K. *Interpretable Visualizations of Data Spaces for Classification Problems* arXiv:2503.05861 [cs]. Mar. 2025. http://arxiv.org/abs/2503.05861.
2. Lin, A., Huguenin-Dumittan, K. K., Cho, Y.-C., Nigam, J. & Cersonsky, R. K. Expanding density-correlation machine learning representations for anisotropic coarse-grained particles.

The Journal of Chemical Physics **161,** 074112. https://doi.org/10.1063/5.0210910 (Aug. 2024).

3. Cersonsky, R. K., Cheng, B., Kofke, D. & Müller, E. A. Machine Learning for Generating and Analyzing Thermophysical Data: Where We Are and Where We're Going. *Journal of Chemical & Engineering Data* **69.** Publisher: American Chemical Society, 2041–2043. https://doi.org/10.1021/acs.jced.4c00207 (June 2024).
4. Gazzarrini, E., Cersonsky, R. K., Bercx, M., Adorf, C. S. & Marzari, N. The rule of four: anomalous distributions in the stoichiometries of inorganic compounds. *npj Computational Materials* **10,** 73. https://www.nature.com/articles/s41524-024-01248-z (Apr. 2024).
5. 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. *Pediatric and Developmental Pathology,* 10935266231197349. http://journals.sagepub.com/doi/10.1177/10935266231197349 (Sept. 2023).
6. 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* **6,** 2480–2487. https://www.sciencedirect.com/science/article/pii/S2590238523003570 (July 2023).
7. 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. https://open-research-europe.ec.europa.eu/articles/3-81/v1 (June 2023).
8. 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. https://www.nature.com/articles/s41524-023-01054-z (June 2023).
9. 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. https://linkinghub.elsevier.com/retrieve/pii/S0143400423000760 (Apr. 2023).
10. 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. http://xlink.rsc.org/?DOI=D2SC06198H (Feb. 2023).
11. Zhou, Y., Cersonsky, R. K. & Glotzer, S. C. A route to hierarchical assembly of colloidal diamond. *Soft Matter* **18,** 304–311. http://xlink.rsc.org/?DOI=D1SM01418H (Jan. 2022).

12. 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. https://iopscience.iop.org/article/10.1088/2632-2153/abfe7c (May 2021).
13. Cersonsky, R. K., Antonaglia, J., Dice, B. D. & Glotzer, S. C. The diversity of three-dimensional photonic crystals. *Nature Communications* **12,** 2543. https://www.nature.com/articles/s41467-021-22809-6 (May 2021).
14. Fraux, G., Cersonsky, R. K. & Ceriotti, M. Chemiscope: interactive structure-property explorer for materials and molecules. *Journal of Open Source Software* **5,** 2117. https://joss.theoj.org/papers/10.21105/joss.02117 (Nov. 2020).
15. 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. https://iopscience.iop.org/article/10.1088/2632-2153/aba9ef (Oct. 2020).
16. Travitz, A., Muniz, A., Beckwith, J. & Cersonsky, R. K. Paper: Bringing Science Education and Research together to REACT, 35030. http://peer.asee.org/35030 (June 2020).
17. 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. https://link.aps.org/doi/10.1103/PhysRevMaterials.2.125201 (Nov. 2018).
18. Cersonsky, R. 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. https://pnas.org/doi/full/10.1073/pnas.1720139115 (Feb. 2018).
19. 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. https://pubs.acs.org/doi/10.1021/acs.jchemed.6b00805 (Sept. 2017).

In Press or Under Review

20. Gazzarini, E., Bercx, M., Cersonsky, R. K., Adorf, C. S. & Marzari, N. Reply to: An explanation for the Rule of Four in Inorganic Materials.
21. Lin, A. Y., Ortengren, L., Hwang, S., Cho, Y.-C., Nigam, J. & Cersonsky, R. K. AniSOAP: Machine Learning Representations for Coarse-grained and Non-spherical Systems. *Journal of Open Source Software*. https://joss.theoj.org/papers/4f031c830d4790cce21dd630588db665 (2025).

Book Chapters

1. Cersonsky, R. K. & De, S. in *Quantum Chemistry in the Age of Machine Learning* 153–181 (Elsevier, Jan. 2023). 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. Censonsky, R. K. *Design Rules for Composites from Resin Transfer Molded Polyimides.* tech. rep. (Tech. Report, UConn and Pratt & Whitney, 2014).
3. Censonsky, 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. Censonsky, 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. Censonsky, 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.
3. Helfrecht, B. A., Censonsky, 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	**Conway Assistant Professorship**, *University of Wisconsin-Madison.*
Jul. 2023	**35 under 35 in Materials Research**, *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**, *UConn.*
2012-2014	**New England Scholar**, *UConn.*
2011	**Babbidge Scholar**, *UConn.*
2010-2014	**Dean's List**, *UConn.*

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	**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) Foundation of Molecular Modeling and Simulation (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.*

Student Awards

Oct. 2024 **Student Presentation Award**, *APS Eastern Great Lakes Section*, Caleb Youngwerth.
Jul. 2024 **Sophomore Research Fellowship**, *UW-Madison*, Caleb Youngwerth.
Mar. 2024 **Travel Award**, *APS Division of Computational Physics (DCOMP)*, Arthur Lin.

Seminars, Conferences, and Workshops

Distinguished Lectures

1. *Chemistry as Data: How We Can Generate Chemical Understanding from Data-Driven Modeling* Keynote Lecture for MRS + Nature (Mar. 2025).
2. *Keynote Lecture: Representation Matters: From Machine Learning for Molecular Simulation to Equity in our Field* University of Connecticut (Sept. 2023).
3. *Victor K. LaMer Award Distinguished Lecture* ACS Colloids (June 2021).
4. *Biointerfaces Innovator Award Lecture* UM (Biointerfaces Institute, Apr. 2019).

Seminars and Invited Lectures

5. *Anisotropic machine learning representations for coarse-graining* Lennard-Jones Centre. Invited Seminar, presented on behalf of R. Cersonsky by Arthur Y. Lin (Oct. 2024).
6. *"Seeing"' Chemical Data through Multi-Objective Lenses* FACSS SciX, Raleigh, North Carolina. Invited Seminar, presented on behalf of R. Cersonsky by Arthur Y. Lin (Oct. 2024).
7. *Late-Breaking Topic: Machine Learning at the Mesoscale: Advances in Analyzing and Coarse-Graining via Data-Driven Approaches* Computational Materials Science and Engineering Gordon Research Conference: The Role of Theories, Simulation, and Machine Learning in Materials Discovery (July 2024).

8. *Invited Speaker: Categorizing three-dimensional photonic crystals: open challenges in scale-covariant problems* CECAM: Machine Learning of First Principles Observables (July 2024).
9. *Representation Matters: "Chemistry as Data" for Machine Learning in Molecular Simulation* Midwest Thermodynamics and Statistical Mechanics Meeting (June 2024).
10. *Invited Seminar* Advancing fluid and soft-matter dynamics with machine learning and data science (June 2024).
11. *Invited Seminar* Department of Chemical Engineering, City University of New York (May 2024).
12. *Machine Learning Force Fields* Institute for Mathematical and Statistical Innovation, University of Chicago (Apr. 2024).
13. *Seminar* Computation and Theory Subgroup, University of Illinois - Urbana/Champaign, Urbana, IL (Feb. 2024).
14. *Invited Speaker, westem* University of Illinois - Urbana/Champaign, Urbana, IL (Feb. 2024).
15. *Seminar, Department of Materials Science and Engineering* Madison, WI (Dec. 2023).
16. *Invited Speaker, The International Symposium on Machine Learning in Quantum Chemistry* Uppsala, Sweden (Nov. 2023).
17. *Invited Speaker, scikit-matter: An Open-Source Suite of Generalizable Machine-Learning Methods Born out of Chemistry and Materials Science* 2023 Machine Learning Interatomic Potential School for Young & Early Career Researchers (Nov. 2023).
18. *Invited Seminar* Trinity College, Dublin (Oct. 2023).
19. *Invited Seminar* American Physical Society - Eastern Great Lakes Section (Oct. 2023).
20. *Disentangling the impact of packing in colloidal and molecular self-assembly* Aberystwyth University, Aberystwyth, UK (Aug. 2023).
21. *Invited Lecture* Iowa State (July 2023).
22. *Machine Learning and Chemistry: Are we there yet?* University of Maryland (May 2023).
23. *Invited Lecture* University of Southhampton (May 2023).
24. *WCPM/HetSys Seminar* University of Warwick, Coventry, UK (Oct. 2022).
25. *WiSFiRE: Women in STEM Frontiers in Research Expo* UConn (Sept. 2022).
26. *Harnessing AI for Design and Understanding Materials Program* Duke University (Sept. 2022).
27. *Modeling Materials at Realistic time Scales via Optimal Exploitation of Exascale Computers and Artificial Intelligence* Iris Adlershof Institute, Berlin, Germany (July 2022).
28. *Marvel Phase 2 Closing Event* SwissTech Convention Center (Apr. 2022).
29. *Marvel Junior Seminar* NCCR Marvel, EPFL (Mar. 2022).
30. *Lennard-Jones Centre Seminar* University of Cambridge, Cambridge, UK (Mar. 2022).
31. *Invited Seminar* University of California, Irvine, Dept. of Materials Science and Engineering (Mar. 2022).

32. *Invited Seminar* University of Minnesota, Chemical Eng. and Materials Science (Feb. 2022).
33. *Invited Seminar* University of Denver, Dept. of Mech. and Materials Engineering (Feb. 2022).
34. *Invited Seminar* Northwestern University, Materials Science and Engineering (Feb. 2022).
35. *Invited Seminar* Boston University, College of Engineering (Feb. 2022).
36. *Invited Lecture* Queen's University (Jan. 2022).
37. *Invited Seminar* University of Wisconsin, Chemical and Biological Engineering (Jan. 2022).
38. *Invited Seminar* Johns Hopkins University, Materials Science and Engineering (Jan. 2022).
39. *Invited Seminar* University of California, Berkeley, Chemical and Biomolecular Engineering (Jan. 2022).
40. *Invited Seminar* University of Amsterdam, AM Lab (Jan. 2022).
41. *Hybrid Unsupervised-Supervised Machine Learning Models for Molecular Science* Statistical Thermodynamics and Molecular Simulations (STMS) (Nov. 2021).
42. *Invited Lecture* University of Michigan (Oct. 2021).
43. *Invited Seminar* US Army DEVCOM Soldier Center (Aug. 2021).
44. *Invited Seminar* Oxford University (Oct. 2018).
45. *Invited Seminar* Eidgenoessische Technische Hochschule (ETH) (Sept. 2018).
46. *Invited Seminar* EPFL (Sept. 2018).

Oral Conference Presentations

47. *A data-driven interpretation of the stability of organic molecular crystals* AIChE Annual Meeting (Nov. 2023).
48. *scikit-matter: An Open-Source Suite of Generalizable Machine-Learning Methods Born out of Chemistry and Materials Science* AIChE Annual Meeting (Nov. 2023).
49. *Expanding Density-Correlation Machine Learning Formalisms for Anisotropic Particles and Hierarchical Systems* AIChE Annual Meeting (Nov. 2023).
50. *Leveraging Machine-Learning for the Structure-Property Paradigm* ACS Colloids and Interfaces, University of North Carolina (June 2023).
51. *A data-driven interpretation of the stability of molecular crystals* APS March Meeting. M28.9 (Mar. 2023).
52. *The Diversity of Three-Dimensional Photonic Crystals for Colloidal Self-Assembly* MRS Annual Meeting. Session BI02 (Dec. 2021).
53. *Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression* MRS Annual Meeting. Session CH04 (Nov. 2021).
54. *The Diversity of Three-Dimensional Photonic Crystals for Colloidal Self-Assembly* AIChE Annual Meeting. 35i (Nov. 2021).
55. *The Search for Novel Mesoscale Materials* AIChE Annual Meeting. 127b (Nov. 2021).

56. *Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression* AIChE Annual Meeting. 203e (Nov. 2021).
57. *Enhanced Machine Learning Models for Structure-Property Mapping with Principal Covariates Regression* APS March Meeting. A60.9 (Mar. 2021).
58. *A New Possibility for Making Diamond Colloidal Crys* AIChE Annual Meeting. 183g, *presented by Yuan Zhou* (Nov. 2020).
59. *Unexpected Photonic Band Gaps in 3D Crystal Structures* APS March Meeting, *Cancelled*. P43.7 (Mar. 2020).
60. *Understanding Photonic Band Gaps in Three Dimensions* AIChE Annual Meeting. 502a (Oct. 2019).
61. *In Search of the Photonic Band Gap* AIChE Annual Meeting. 455c, *presented by S. C. Glotzer* (Oct. 2019).
62. *Can we design a reconfigurable photonic crystal in the visible light range?* APS March Meeting. C50.7 (Mar. 2019).
63. *Pressure–Tunable Photonic Band Gaps in an Entropic Colloidal Crystal* MRS Fall Meeting. Session BM03 (Nov. 2018).
64. *Pressure–Tunable Photonic Band Gaps in an Entropic Colloidal Crystal* AIChE Annual Meeting. 276c (Oct. 2018).
65. *Tunable Photonic Band Gaps in an Entropic Crystal* Anisotropic Particles Symposium, Konstanz, Germany (Sept. 2018).
66. *Tunable Photonic Band Gaps in an Entropic Crystal* Self-Assembly of Colloidal Systems, Bordeaux, France (Sept. 2018).
67. *Tunable Photonic Band Gaps in an Entropic Crystal* APS March Meeting. H12.12 (Mar. 2018).
68. *Insights into Inverse Materials Design from Phase Transitions in Shape Space* AIChE Annual Meeting. 704f (Nov. 2017).
69. *Insights into Inverse Materials Design from Phase Transitions in Shape Space* MRS Meeting. CM3.3.05/CM7.2.05, *2nd Place Prize* (Apr. 2017).
70. *Augmenting Primary and Secondary Education with Polymer Science and Engineering* ACS Meeting (Apr. 2017).
71. *Insights into Inverse Materials Design from Phase Transitions in Shape Space* APS March Meeting. C17.02 (Mar. 2017).

Poster Presentations

72. *Harnessing the Data Revolution (HDR) at NSF* (Oct. 2023).
73. *Foundations of Molecular Modeling and Simulation* Delavan, WI (July 2022).
74. *MRS Fall Meeting* Boston, MA. poster in Session EL01, poster Award (Dec. 2019).
75. *Foundations of Molecular Modeling & Simulation* Delavan, WI. poster (July 2018).

76. *When don't colloids order into cubic-close packings?* APS March Meeting. L60.144, *presented by S. Barterian* (Mar. 2018).
77. *Macromolecular Science and Engineering Symposium* UM, Ann Arbor, MI. poster (Oct. 2017).
78. Engineering Graduate Symposium. poster, *3rd Place Prize* (Nov. 2016).
79. *Macromolecular Science and Engineering Symposium* UM, Ann Arbor, MI. poster (Oct. 2016).
80. *Michigan Institute for Computational Discovery and Engineering Symposium* UM, Ann Arbor, MI. poster, *3rd Place Prize* (Apr. 2016).
81. *Macromolecular Science and Engineering Symposium* UM, Ann Arbor, MI. poster, *1st Place Prize* (Oct. 2015).
82. *Soft Matter Summer School* University of Massachusetts. poster (June 2015).

Student Conference Presentations

5. *Anisotropic machine learning representations for coarse-graining* Lennard-Jones Centre. Invited Seminar, presented on behalf of R. Cersonsky by Arthur Y. Lin (Oct. 2024).
6. *"Seeing"' Chemical Data through Multi-Objective Lenses* FACSS SciX, Raleigh, North Carolina. Invited Seminar, presented on behalf of R. Cersonsky by Arthur Y. Lin (Oct. 2024).
83. *Determining the Limit of Extrapolation for Macromolecular Machine Learning Potentials* APS March Meeting, Minneapolis, MN. Presenter: Natalie Hooven (Mar. 2024).
84. *Anisotropic Machine Learning Representations for Multiscale Systems* APS March Meeting, Minneapolis, MN. Presenter: Arthur Y. Lin (Mar. 2024).

Synergistic Activities

Teaching

Courses Taught at UW-Madison

Spring 2023 **CBE 440**, *Chemical Engineering Materials.*
Fall 2023 **CBE 710**, *Advanced Chemical Engineering Thermodynamics.*
Spring 2024 **CBE 440**, *Chemical Engineering Materials.*
Fall 2024 **CBE 710**, *Advanced Chemical Engineering Thermodynamics.*

Courses and Workshops outside UW-Madison

Jul. 2023 **Unsupervised Learning, Data Management**, *i-COMSE Workshop on Machine Learning for Molecular Simulation*, Minneapolis, MN.

Mentorship and Supervision of Junior Researchers

Undergraduate Researchers

2023–2024 **Yong-Cheol Cho**, *UW CBE and CSE*, Accelerating `AniSOAP` via caching and compile languages. *Pub. in [2] and [21].*
PhD student at the University of Illinois - Urbana/Champaign.

2023– **Caleb Youngwerth**, *UW Physics*, Exploring the phase space of colloidal particles in ionic liquids.

2023–2024 **Seungmin (Henry) Lee**, *UW CBE*, Crystallographic categorizations of photonic crystals, *Pub. in [0]*.
PhD student at Notre Dame University

2023–2024 **Anna Claire Crowley**, *UW CBE.*

2023– **Natalie Hooven**, *UW CBE*, Determining the limit of extrapolation for macromolecular machine learning potentials. *Presented by NH at 2024 APS*, *Pub. in [0]*.

2023– **Lucas Ortengren**, *UW Physics*, Documentation for `AniSOAP`, *Pub. in [21]*.

2023– **Seonwoo Hwang**, *UW CBE*, *Pub. in [21]*.
On leave for mandatory military service

2024– **Matthew Reutemann**, *UW CBE*, Melting simulations for heterocyclic hydrogen carriers.

2024 **Trystan McCaskill**, *Howard University Chemical Engineering*, *NSF REU*, Computing relaxation times for glassy dynamics.

Graduate Researchers

2022– **Arthur Lin**, *UW CBE*, `AniSOAP`, a machine-learning framework for data-driven coarse-grain simulation. *Pubs. in [1, 21, 2]* .

2022–2024 **Saswat Kumar Nayak**, *UW CBE MS*, Topological descriptors in strictly periodic systems, *Pub. in [0]*.

2023– **Hwigwang Lim**, *UW CBE*, Designing colloidal gel networks for mechanical support of neat ionic liquid electrolytes.

2023– **Charles Carroll**, *UW CBE*, Glassy behavior in organic molecules, role of local symmetry and topology.

2023– **Christian Jorgenson**, *UW CBE*, Crystal structure prediction of flexible organic molecules for pharmaceutical design. *Pub. in [1]*.

2024– **Ethan Deutsch**, *UW CBE*, Topological analyses of glassy systems, co-advised with Victor Zavala.

Advisees prior to 2023

2021-2023 **Victor Principe**, *PhD Student, EPFL IMX*, Approximating the Landscape of Molecular Crystals for NMR Shielding Predictions, *Pub. in ORE [7]*.
Currently: Battery Consultant at Sphere Energy

2020-2022 **Sergei Kliavinek**, *Semester Project Student, EPFL IMX*, Comparing Feature Spaces for Small Molecules. *Pubs. in MLST [12] and ORE [7]*.
Currently: 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.
Currently: Analytics Consultant at ESPOO

2020-2021 **Maria Pakhnova**, *Project Inspire Student, EPFL IMX*, Identifying High-Stability Components of Molecular Crystals. *Pub. in Chem. Sci. [10]*.

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, *Pubs. in MLST [15], [12], and ORE [7]*.
Currently: Postdoctoral Reseacher at Pacific Northwest National Laboratory

2018-2020 **Yuan Zhou**, *PhD Student, UM ChE*, A new possibility for making diamond colloidal crystals. *Pub. in Soft Matter[11]*.
Currently: Data Scientist with Huawei

2016-2018 **Alyssa Travitz**, *PhD Student, UM Macro*, Mentored through UM Mentorship Program, *Pub. in ASEE [16]*.
Currently: 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*.
Currently: Assistant Audio Engineer at Iyuno-SDI Group

Professional Service

Professional Organization Service

2025 **CECAM: Machine Learning for Materials Prediction**, *Organizing Team.*

2025 **Midwest Thermodynamics & Statistical Mechanics Meeting**, *Lead Organizer.*

2024–present **Liaison Director**, *AIChE Computational Molecular Science & Engineering Forum.*

2024 **APS March Meeting**, *Conference Session Organizer, Advances in Macromolecular Simulation and Modeling.*

2024 **ACS Annual Meeting**, *Conference Session Organizer, Unsupervised Techniques: Theory and Applications.*

2024 **Discussion Leader: Power Hour**, *Gordon Research Conference on Computational Materials Science and Engineering.*

2023–present **Fall Programming Chair**, *AIChE Women in Chemical Engineering (WIC).*

Journal Editorship

2024–present **Editorial Board, Machine Learning: Science and Technology**.

2025 **Guest Editor, Journal of Chemical Theory and Computation**, *Machine Learning and Statistical Mechanics: Shared Synergies for Next Generation of Chemical Theory and Computation.*

2024 **Guest Editor, Journal of Chemical and Engineering Data**, *Machine Learning of Thermophysical Properties*, https://pubs.acs.org/page/jceaax/vi/jcedml2024.

Department Committees: Climate and Inclusion (2023 -), Graduate Admissions (2023), Personnel (2024 -), PhD Program (2024 -), Graduate Recruiting (2024 -)

Journal Peer Review: 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, Scientific Reports

Proposal Peer Review: NSF, National Academies of Science, Engineering, and Medicine

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.

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.