

Michael Tynes

Vitae

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Education

- 2022–Present **University of Chicago**, Ph.D., Department of Computer Science, DOE CSGF Fellow. Advisor: Dr. Ian Foster
- 2018–2020 **Fordham University**, M.S. Data Science, Department of Computer and Information Science, GPA: 4.0
Honor's Thesis: *Tensor Factorizations for Recommending Perovskite Crystal Trials*
- 2013–2017 **Fordham University**, B.S. Psychology, (Minor in Philosophy),
Major GPA: 4.0 (Overall: 3.8, *summa cum laude*)
Honor's Thesis: *Hair Cortisol: Associations with Perceived Stress and Salivary Diurnal Cortisol*

Research Interests

- ML for Scientific Research
- ML Algorithm Development
- Scientific Data Infrastructure
- Interpretable ML
- Domain-informed ML
- Autonomous Discovery Algorithms

Selected Experience

- 2022–Present **Graduate Research Assistant**, The University of Chicago, Department of Computer Science
- 2020–2022 **Post Masters Research Fellow**, Los Alamos National Laboratory, T-1: Physics of Chemistry and Materials
- Developed methods to improve accuracy, interpretability, and cost of ML for chemical property prediction
 - Designed and ran machine learning experiments on LANL and DOE supercomputers
 - Developed software for autonomous machine-learning-driven chemical robotics
 - Contributed to the cinema data visualization toolkit
- 2018–2020 **Graduate Research Assistant**, Fordham University, Departments of Computer Science and Chemistry
- Developed tensor-factorization-based chemical reaction recommendation algorithms
 - Conducted machine learning experiments at the Texas Advanced Computing Center
 - Built software and user interfaces for the open source ESCALATE laboratory automation tool
- 2016–2018 **Research Coordinator and Laboratory Manager**, Fordham University, Departments of Psychology and Chemistry
- Lead execution of a multi-stage psychological study with hundreds of participants
 - Automated data integration across modalities including physiological sensor signals, hormone measurements, cognitive tests, and the US Census
 - Headed a team of over fifteen graduate, undergraduate, and high school students

- Built laboratory pipeline for hormone quantification in human hair and saliva

Selected Coursework

Algorithms, Data Mining, Software Engineering, Big Data Programming, Deep Learning, Reinforcement Learning, Optimization Methods, Computational Chemistry

Skills and Technologies

Python (scipy stack, django), Parallel Python (dask, joblib, multiprocessing) R (base-r, tidyverse), MATLAB, Mathematica, Unix/Linux, Slurm, PostgreSQL, MongoDB

Awards and Honors

- 2022-2026 **DOE Computational Science Graduate Fellowship (CSGF)**, Full support for four years of Ph.D. studies (8% acceptance)
- 2021-2022 **LANL Seaborg Fellowship**, Award to support interpretable machine learning for autonomous discovery in Actinide science (25% acceptance)
- 2021-2022 **LANL ISTI Fellowship**, Award to support development of software infrastructure for autonomous discovery in laboratory science at LANL
- 2020-2021 **LANL CNLS Fellowship**, Award to support the development of Pairwise Difference Regression (PADRE)
- 2019-2020 **Fordham GSAS Graduate Research Fellowship**, Funding to support development of tensor factorization based reaction recommendation systems in chemical science. Funded by Fordham GSAS and the DARPA SD2 program (PI: Joshua Schrier)
- 2018-2019 **Fordham Centennial Graduate Research Fellowship**, Funding from Fordham GSAS granted to the top 10% of students admitted to the MSDS program
- 2017 **Fordham James C Higgins Memorial Award in Psychology**, (Fordham College at Rose Hill), One of three named awards given annually to a graduating senior for distinguished performance and contributions to the department
- Fall 2016 **Fordham Undergraduate Research Grant**, Continued research support from Fordham College at Rose Hill for hormone quantification pipeline development
- Summer 2016 **Fordham Undergraduate Research Grant**, Initial research support from Fordham College at Rose Hill for hormone quantification pipeline development

Publications

Peer-reviewed articles

- [1] **Tynes, M.**, Gao, W., Burrill, D.J. Batista, E.R., Perez, D., Yang, P., and Lubbers, N. "Pairwise difference regression for uncertainty quantification and candidate selection." *Journal of Chemical Information and Modelling*. 61, 8, 3846–3857 (2021). (2019 IF: 4.5) <https://doi.org/10.1021/acs.jcim.1c00670>
- [2] Schrier, J., **Tynes, M.**, and Cain, L. "Determining the Activity Series with the Fewest Experiments using Sorting Algorithms" *Journal of Chemical Education*. 98, 5, 1653–1658 (2021). (2019 IF: 1.7) <https://doi.org/10.1021/acs.jchemed.1c00043>

- [3] Yip, T., Smith, P., **Tynes, M.**, Mirpuri, S., Weems, A., and Cheon, Y. M. "Discrimination and hair cortisol concentration among asian, latinx and white young adults." *Comprehensive Psychoneuroendocrinology*. 6, 100047 (2021). (2019 IF: 4.7) <https://doi.org/10.1016/j.cpniec.2021.100047>
- [4] Pendleton, I.M., Caucci, M.K., **Tynes, M.**, Dharna, A., Nellikkal M.A., Li, Z., Chan E.M., Norquist, A.J., and Schrier, J. "Can Machines "Learn" Halide Perovskite Crystal Formation without Accurate Physicochemical Features?" *Journal of Physical Chemistry C*. 124, 25, 13982–13992 (2020). (2019 IF: 4.2) <https://doi.org/10.1021/acs.jpcc.0c01726>
- [5] Jones, L., **Tynes, M.**, and Smith, P. "Prediction of models for ordered solvent in macromolecular structures by a classifier based upon resolution-independent projections of local feature data." *Acta Crystallographica Section D: Structural Biology*. 75, 8, 696-717 (2019). (2019 IF: 7.7) <https://doi.org/10.1107/S2059798319008933>
- [6] Zheng, W., **Tynes, M.**, Gorelick, H., Mao, Y., Cheng, L., and Hou, Y. "Flow-Con: Elastic Flow Configuration for Containerized Deep Learning Applications." *Proceedings of the 48th International Conference on Parallel Processing* Article 87, 1-10 (2019). (Conference Acceptance Rate: 20%) <https://doi.org/10.1145/3337821.3337868>

Conference presentations

- [1] **Tynes, M.** and Schrier, J. "How to GET novel perovskites: using the ESCALATE open source laboratory automation tool's REST API to drive the discovery of materials" *A Virtual Workshop on Autonomous Discovery in Science and Engineering*. Center for Advanced Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Laboratory. Berkeley, CA. April 21, 2021.
- [2] **Tynes, M.** and Schrier, J. "Tensor factorization for automated materials discovery based on data from failed experiments." Poster presented at *AI and Tensor Factorizations for Physical, Chemical, and Biological Systems*. Center for Nonlinear Studies (CNLS), Los Alamos National Laboratory. Santa Fe, NM. September 18, 2019.
- [3] **Tynes, M.**, Hoyt, L., and Smith, P. "Testing the convergence of biological indices of chronic stress: hair and diurnal cortisol." Presentation delivered at *The National Council of Undergraduate Research*. Memphis, TN. April 7, 2017
- [4] **Tynes, M.** Akhter, F., Sullivan, M., Yip, T., Smith, P. "Hair Cortisol Analysis as a Measure of Discrimination-Associated Chronic Stress." Poster presented at *The Biennial meeting of the American Psychological Association, Division 45* Palo Alto, CA. July 7, 2016.

References

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