Joshua A. Rackers
Machine Learning Scientist
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Education

Washington University in St. Louis	Computational Biophysics	Ph.D. 2019
Johns Hopkins University	Urban Education	M.S. Ed. 2012
Ohio State University	Physics and Political Science	B.S. 2010

Employment

Prescient Design / Genentech	Machine Learning Scientist	2022-present
Sandia National Laboratories	Truman Fellow	2019-2022
Washington University in St. Louis	Graduate Research Assistant	2013-2019
Baltimore City Public Schools	Physics and Chemistry Teacher	2010-2013

Teaching, Mentoring and Service

UC Berkeley Data Science Discovery Program: Fall 2023

Mentoring a small group of undergraduate students. The students are taking on the challenge of building machine learning (ML) models for quantum chemistry in drug discovery. In addition to teaching the basics of machine learning research tools, I am leading them on an exploration of the frontiers of 3D equivariant ML methods.

Prescient Design DEI Working Group

I co-lead a small group with a mandate to improve diversity, equity, and inclusion (DEI) in the organization. We lead a DEI book club and organize a forum for advancing policy changes to address systemic inequities.

Mentorship @ Prescient Design: 2023-present

- Bodhi Vani: Machine Learning Scientist, and my first direct report. Bodhi is working on building physics-informed ML models for molecular dynamics.

Mentorship @ Sandia National Laboratories: 2019-2022

- Shivesh Pathak: Postdoctoral Fellow. Shivesh worked on building quantum chemistry methods to generate data for ML electron density models.
- Alex Lee: Postdoctoral Fellow (joint with University of New Mexico). Alex worked on applying ML electron density methods to DNA.
- Pranav Rao: Summer Intern. Pranav investigated the “unreasonable effectiveness” of equivariant neural networks for 3D learning tasks.
- Alexander Muñoz: Summer Intern. Alex contributed to the understanding of unstable training dynamics of equivariant neural networks.
- Lucas Tecot: Intern. Lucas contributed to our foundational ML electron density work.

- Roseane Silva: Graduate Student (formally mentored by Jay Ponder). Roseane undertook developing the HIPPO model I invented into a model for general simulations.

Science Club with Mr. Rackers: 2014-2018

Led a weekly, after-school science club for 4th and 5th grade students at Patrick Henry Elementary School in St. Louis Public Schools.

Honors and Awards

Bay Area Research SLAM Finalist	"Mapping the Quantum World with Machine Learning"	2021
Sandia Postdoctoral Showcase	First Place	2020
Sandia ACORN Project ($200k over 2 years)	Machine Learning DNA Electron Densities	2020
Sandia LDRD Truman Fellowship ($900k over 3 years)	Next Generation Methods for Simulating Biomolecules	2019
Cecil M. DeGutis Prize in Chemical Biology	Washington University in St. Louis Medical School	2019
NSF Molecular Sciences Software Institute (MOLSSI) Fellowship	Development of Biomolecular Molecular Dynamics Models	2018
MilliporeSigma Fellowship in Memory of Dr. Gerty Cori	Predoctoral Fellowship	2013
Teach For America Baltimore	Future School Leaders Fellowship	2012

Publications

- Pinheiro, P. O., **Rackers, J. A.,** Kleinhenz, J., Maser, M., Mahmood, O., Watkins, A. M., ... & Saremi, S. (2023). 3D molecule generation by denoising voxel grids. *arXiv preprint arXiv:2306.07473*.
- **Rackers, J. A.,** Tecot, L., Geiger, M., & Smidt, T. E. (2023). A recipe for cracking the quantum scaling limit with machine learned electron densities. *Machine Learning: Science and Technology*, *4*(1), 015027.
- Pathak, S., López, I. E., Lee, A. J., Bricker, W. P., Fernández, R. L., Lehtola, S., & **Rackers, J. A.** (2023). Accurate Hellmann–Feynman forces from density functional calculations with augmented Gaussian basis sets. *The Journal of Chemical Physics*, *158*(1).
- Lee, A., **Rackers, J. A.,** Pathak, S., & Bricker, W. (2023). Building an ab initio solvated DNA model using Euclidean neural networks. *ChemRxiv preprint*
- Lee, A. J., **Rackers, J. A.,** & Bricker, W. P. (2022). Predicting accurate ab initio DNA electron densities with equivariant neural networks. *Biophysical Journal*, *121*(20), 3883-3895.
- **Rackers, J. A.,** & Rao, P. (2022). Hierarchical Learning in Euclidean Neural Networks. *arXiv preprint arXiv:2210.04766*.

- Chung, M. K., Wang, Z., **Rackers, J. A.,** & Ponder, J. W. (2022). Classical Exchange Polarization: An Anisotropic Variable Polarizability Model. *The Journal of Physical Chemistry B*, *126*(39), 7579-7594.
- Koski, J. P., Moore, S. G., Clay, R. C., O'Hearn, K. A., Aktulga, H. M., Wilson, M. A., **Rackers, J. A.,** ... & Modine, N. A. (2021). Water in an external electric field: comparing charge distribution methods using ReaxFF simulations. *Journal of Chemical Theory and Computation*, *18*(1), 580-594.
- **Rackers, J. A.,** Silva, R. R., Wang, Z., & Ponder, J. W. (2021). Polarizable Water Potential Derived from a Model Electron Density. *Journal of Chemical Theory and Computation, 17*(11), 7056-7084.
- Jing, Z., **Rackers, J.A.,** Pratt, L., Liu, C., Rempe, S., Ren, P. (2021). Thermodynamics of ion binding and occupancy in potassium channels. *Chemical Science, 12*(25), 8920-8930.
- **Rackers, J.A.** & Ponder, J.W. (2019). Classical Pauli Repulsion: An Anistropic, Multipole Model. *The Journal of Chemical Physics*, 150(8), 084104.
- **Rackers, J. A.,** Liu, C., Ren, P., & Ponder, J. W. (2018). A physically grounded damped dispersion model with particle mesh Ewald summation. *The Journal of chemical physics*, *149*(8).
- **Rackers, J. A.,** Wang, Z., Lu, C., Laury, M. L., Lagardere, L., Schnieders, M. J., ... & Ponder, J. W. (2018). Tinker 8: software tools for molecular design. *Journal of Chemical Theory and Computation*, *14*(10), 5273-5289.
- **Rackers, J. A.,** Wang, Q., Liu, C., Piquemal, J. P., Ren, P., & Ponder, J. W. (2017). An optimized charge penetration model for use with the AMOEBA force field. *Physical Chemistry Chemical Physics*, *19*(1), 276-291.
- Narth, C., Lagardere, L., Polack, É., Gresh, N., Wang, Q., Bell, D. R., **Rackers, J. A.** ... & Piquemal, J. P. (2016). Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. *Journal of computational chemistry*, *37*(5), 494-506.
- Wang, Q., **Rackers, J. A.,** He, C., Qi, R., Narth, C., Lagardere, L., ... & Ren, P. (2015). General model for treating short-range electrostatic penetration in a molecular mechanics force field. *Journal of chemical theory and computation*, *11*(6), 2609-2618.

Selected Invited Talks

- Nvidia Computational Drug Discovery Group: "Building physics into AI for structure-based drug design", 2023
- UNM Center for Quantum Information and Control: "How we can use machine learning to discover new physics", 2022
- Swiss Equivariant Learning Workshop: "Beyond the Black Box: The potential and problems of equivariant models", 2022

- Tinker Developers Meeting: “Implementing polarizable force fields in LAMMPS”, 2022
- Telluride Science Research Center Workshop: “Combining physics and machine learning to tackle the next generation of problems in biomolecular modeling”, 2022
- CECAM Workshop on Non-Covalent Interactions in Large Molecules: “Probing the extent of electron correlation in biomolecules with machine learning”, 2021
- LAMMPS Workshop: “What can you do with a polarizable force field?”, 2021
- DOE Computing Research Leadership Council Series, 2021
    a. University of Washington
    b. University of Texas at El Paso
    c. San Diego State University
- University of New Mexico Department of Biology: “Predicting the behavior of biomolecules with physics and machine learning”, 2020
- NSF MolSSI Workshop: “HIPPO: A polarizable, atomic density-based model for water”, 2019
- Tinker Developers Workshop: “AMOEBA 2.0 Software Implementation”, 2018
- Gordon Research Conference on Computational Aspects – Biomolecular NMR: “AMOEBA 2.0, a physics-first approach to biomolecular simulation”, 2017
- National Institutes of Health Laboratory of Computational Biophysics: “Short-range electrostatics and the grand challenge of biophysics”, 2016