**Joshua A. Rackers**
Machine Learning Scientist and Group Leader
Prescient Design / Genentech
joshrackers@gmail.com
joshrackers.owlstown.net

## Education

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|---|---|---|
| *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

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| *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 took 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 lead 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. Bodhi is working on building physics-informed ML models for molecular dynamics.
- Ameya Daigavane: Summer Intern. Ameya worked on developing equivariant models for generative AI models for molecular dynamics.
- Ewan Wallace: Apprentice at Roche Informatics. Ewan is building ML models for quantum chemistry.

*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

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| *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

- Wang, Y., Takaba, K., Chen, M. S., Wieder, … **Rackers, J. A.,** … & Tuckerman, M. E. (2024). On the design space between molecular mechanics and machine learning force fields. arXiv preprint arXiv:2409.01931.
- O Pinheiro, P. O., **Rackers, J. A.,** Kleinhenz, J., Maser, M., Mahmood, O., Watkins, A., … & Saremi, S. (2024). 3D molecule generation by denoising voxel grids. Advances in Neural Information Processing Systems, 36.
- Lee, A. J., **Rackers, J. A.,** Pathak, S., & Bricker, W. P. (2024). Building an ab initio solvated DNA model using Euclidean neural networks. Plos one, 19(2), e0297502.
- **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. 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**

- Telluride Science Research Center Workshop: “Can AI algorithms learn many-body interactions? Lessons from a journey in drug discovery.”, 2024
- 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