

John Parkhill

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Machine learning leader in AI-driven drug discovery. Founded Terray Therapeutics' ML function and grew it to a nine-person team whose generative, structural, and agentic models run the company's design-make-test-analyze loop. More than a decade leading research teams across biotech, a macro fund, and academia; NSF CAREER awardee with 30+ peer-reviewed publications, 7,800+ citations, and an h-index of 25.

experience

2022 – Present **DIRECTOR OF MACHINE LEARNING** *Terray Therapeutics*

- Founded Terray's ML function; recruited and lead a nine-person team of ML researchers and engineers, owning strategy, roadmap, hiring, and the model portfolio in partnership with medicinal chemistry, biology, and engineering
- Built the model stack behind Terray's design-make-test-analyze engine: multi-property Bayesian optimization, synthesizability, and ADME models that propose and prioritize candidate molecules in every weekly design cycle (2025 [🔗](#))
- Built Terray's tool-using agent harness and the agentic loops on it, spanning laboratory data, hypothesis generation, day-to-day research assistance for scientists, and an autonomous design loop that discovered cellularly active (<20 nM) inhibitors of an immunology target in two months
- Lead a vision-language model (VLM) collaboration with NVIDIA: fine-tuned Nemotron VLMs that set a new state of the art for parsing chemical reaction diagrams from the literature (2026 [🔗](#))
- Led pretraining of transferable co-posing and potency models for protein–ligand complexes, validated against prospective experimental outcomes rather than published benchmarks (ICML 2026 [🔗](#))
- Developed a multimodal generative equivariant transformer for 3D molecular design (JCIM 2023 [🔗](#)) and a latent diffusion scheme for controlled molecule generation (2024 [🔗](#))
- Ship the production inference services and interactive design interfaces used daily by the medicinal chemistry team; run distributed training and inference across multi-node NVIDIA DGX, AWS, Lambda Labs, and Modal

2018 – 2022 **HEAD OF QUANTITATIVE RESEARCH** *Artemis Capital Management*

Led research and data operations for a long volatility fund

- Hired and managed a four-person quantitative research team and set its research agenda
- Put ML into production on live capital: neural stochastic differential equation models of volatility surfaces that screened trades and sized risk for the trading desk
- Implemented index spread quantitative arbitrage strategies with a measured Sharpe ratio above 2
- Designed and ran the fund's data platform: AWS microservices, ETL pipelines, a price database spanning millions of instruments (CBOE, CME, OPRA), and the interactive tools that delivered signals to traders

2013 – 2018 **ASSISTANT PROFESSOR** *University of Notre Dame*

Led a research group in machine learning and quantum electronic dynamics; NSF CAREER Award (2018)

- Created TensorMol, an open-source neural network model of chemistry with long-range physics (Chem. Sci. 2018, 600+ citations [🔗](#)), and neural models of bond energies covered in Chemistry World ([🔗](#))
- Pioneered machine-learned orbital-free density functional theory: a convolutional neural network kinetic energy functional of the electron density that reproduces Kohn–Sham potential energy surfaces without orbitals (JCTC 2016, 150+ citations [🔗](#))
- Developed self-consistent models of electronic dynamics and relaxation (the CAREER project) and, with experimental collaborators, explained the size-dependent Stokes shift in CsPbBr₃ perovskite nanocrystals (JACS 2017, 390+ citations [🔗](#))
- Trained and mentored Ph.D. students in tensor frameworks and neural models; 13 publications including PNAS and the Journal of the American Chemical Society

education

2010 – 2013 **POSTDOCTORAL FELLOW** *Harvard University*

Quantum electronic dynamics with Alán Aspuru-Guzik; 6 publications [🔗](#)

2006 – 2010 **PH.D. QUANTUM CHEMISTRY** *University of California, Berkeley*

Thesis: Local Models of Strongly Correlated Systems ([🔗](#)); 10 publications; contributor to the Q-Chem package [🔗](#)

2001 – 2005 **B.S. MATHEMATICS AND CHEMISTRY** *University of Chicago*

With honors; Norman H. Nachtrieb Award in Chemistry; Pfizer Fellowship

skills

Machine Learning: PyTorch, JAX, Hugging Face, transformers, diffusion and equivariant/graph models, Bayesian optimization, active learning, uncertainty quantification, LLM agents and tool use

Systems: Python, C++, CUDA, distributed training, vLLM, Docker, Kubernetes, AWS, Modal, Lambda Labs, NVIDIA DGX, microservices, ETL, SQL