

Leandro Seixas Rocha, PhD

Machine Learning Engineer | Scientific ML & Deep Learning | PyTorch, Python/C++ | High-Performance Computing

Ilum – School of Science

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Summary

Machine Learning Engineer & Computational Scientist with a Ph.D. in Physics and 10+ years of international R&D experience (Brazil, US, Singapore). Specialized in AI for Science and Scientific Machine Learning (SciML), bridging deep learning (GNNs, Neural Operators) with physics-based modeling to accelerate large-scale simulations and high-throughput workflows. Proficient in Python, PyTorch, C++, and HPC environments, with a proven track record of designing open-source scientific software, deploying end-to-end ML pipelines, and leading multidisciplinary engineering and research initiatives.

Work Experience

CNPEM (2026 – Present)

CAMPINAS, SP, BRAZIL

Research Fellow

- Developed **deep learning frameworks** to predict fundamental electronic properties (electron charge and kinetic energy densities) using **Fourier Neural Operators (FNOs)** and highly interpretable symbolic regression.
- Engineered large-scale data pipelines to process terabytes of materials data across thousands of crystal structures and chemical compounds.
- Achieved up to a 50x computational speedup in calculating electronic properties compared to conventional first principles (DFT) methods.

IFT/UNESP (2025)

SÃO PAULO, SP, BRAZIL

Research Fellow

- Engineered machine learning models for nanoscale systems, implementing **Graph Neural Networks (GNNs)** to predict total energies and interatomic forces with quantum-level accuracy.
- Optimized distributed training workflows for large-scale model convergence and efficient resource utilization on computing clusters.
- Scaled molecular dynamics simulations by 100x, enabling dynamic property evaluations of complex systems far beyond the size limits of standard quantum calculations.

MACKENZIE PRESBYTERIAN UNIVERSITY (2016 – 2024)

SÃO PAULO, SP, BRAZIL

Assistant Professor

- Taught undergraduate and graduate courses in Python, C++, solid-state physics, thermodynamics, and nanomaterials.
- Spearheaded technical direction and mentored a multidisciplinary team of up to 15 Ph.D. researchers and graduate students while successfully securing competitive R&D grant funding.
- Integrated quantum mechanical modeling with machine learning (e.g., **Gradient Boosting**) to interpret, predict, and guide experimental laboratory discoveries.
- Accelerated the screening and design of novel nanomaterials for next-generation energy storage (batteries), green hydrogen generation, and optical communication devices.

NATIONAL UNIVERSITY OF SINGAPORE (2014 – 2015)

SINGAPORE, SINGAPORE

Research Fellow

- Formulated computational and effective analytical models to investigate and explain electronic and optical phenomena in low-dimensional nanomaterials.
- Conducted high-throughput ab initio simulations leveraging **High-Performance Computing** (HPC) environments and quantum mechanical solvers.
- Pioneered the discovery of a novel class of 2D multiferroic materials (coupling magnetic and elastic order), resulting in a featured publication in a high-impact peer-reviewed journal.

RENSSELAER POLYTECHNIC INSTITUTE (2012 – 2013)

TROY, NY, USA

Research Assistant

- Modeled interfacial electronic structures between semiconductors and topological insulators using quantum mechanical methods.
- Derived effective Hamiltonian models to capture emergent electronic couplings and interfacial boundary physics.
- Discovered the spin-texture proximity effect, delivering fundamental mechanisms and theoretical benchmarks for advanced spintronics and quantum computing architectures.

Skills (Selected)

Python | C++ | PyTorch | scikit-learn | XGBoost | Optuna | Neural Operators | Symbolic regression | Machine Learning Interatomic Potentials (MLIP) | Graph Neural Networks (GNNs) | ASE | VASP | Siesta | Quantum ESPRESSO | GPAW | ORCA | NumPy | SciPy | Pandas | PyPI | GitHub | Linux | MPI | Slurm | HPC

Projects (Selected)

PORAQUÊ < <https://poraque.seixas.dev> >

An open-source Python framework for machine learning in electronic structure calculations.

MANDACARU < <https://mandacaru.seixas.dev> >

An open-source Python framework for electronic structure calculations using classical and quantum computing methods to generate data for ML pipelines.

QUASIGRAPH < <https://github.com/seixas-research/quasigraph> >

An open-source toolkit designed for generating chemical and geometric descriptors to be used in machine learning models.

Education

PhD, Physics (2009 – 2014)

University of São Paulo (USP), São Paulo, SP, Brazil

M.Sc., Physics (2007 – 2009)

Federal University of ABC (UFABC), Santo André, SP, Brazil

B.Sc., Physics (2003 – 2007)

Federal University of Paraíba (UFPB), João Pessoa, PB, Brazil

Languages

English: Full professional proficiency

Portuguese: Native