

Adrian Domínguez Castro, Ph.D.

Machine Learning Researcher | AI for Science

[Email](#) · [Linkedin](#) · [GitHub](#) · [Google Scholar](#) · [Website](#)

SELECTED EXPERIENCE

Data Scientist | Machine Learning · Apr 2024-Present

ADC Scientific Consulting, USA.

Selected engagements:

Decimal.health - Venture Studio (AccelerOnc Studio, Moffitt Cancer Center)

- Architected and implemented end-to-end RAG search systems for clinical and scientific datasets, optimizing vectorization and retrieval strategies for high-dimensional data
- Engineered automated data pipelines for scientific data management, ensuring high-fidelity ingestion and data integrity for LLM-based discovery
- Developed agentic workflows using LangGraph to automate high-fidelity data ingestion and scientific reasoning processes.

Postdoctoral Research Scientist · Feb 2023-Jan 2024

Vanderbilt University, USA

- Led a project integrating DFT and Machine Learning to predict catalytic material properties with over 85% accuracy, resulting in a peer-reviewed publication. [Link](#)
- Implemented computational chemistry simulations and developed Python scripts to automate data collection and processing, enhancing efficiency by 80%.

Doctoral Research Scientist · Oct 2018-Dec 2022

University of Bremen, Germany

- Led 3+ multi-year research projects, resulting in 4 peer-reviewed publications and developed data science solutions resulting in a 50% reduction of processing time.
- Directed data modeling and advanced simulations for computational chemistry, machine learning delivering insights in 10+ talks at scientific meetings. Built and led interdisciplinary teams, fostering collaborations across five countries (Germany, Spain, China, USA, and France)

EDUCATION

Ph.D. in Physics (Dr. rer. nat., Germany) · 2022 · University of Bremen, Germany

B.Sc. in Radiochemistry · 2014 · InSTEC-University of Havana, Cuba

SKILLS

- Machine Learning & Deep Learning
- LLMs & RAG
- LangGraph
- Linux & HPC
- Programming: Python, C/C++
- Quantitative Research
- Data Science
- Statistics & Predictive Analytics
- Computational Chemistry
- Project Management

CERTIFICATIONS

- **Deep Learning Specialization** by Stanford University & DeepLearning.AI on Coursera.
- **Machine Learning Specialization** by Stanford University & DeepLearning.AI on Coursera.
- **ChatGPT Prompt Engineering for Developers** by DeepLearning.AI on Coursera.
- **AI for Everyone** by Stanford University & DeepLearning.AI on Coursera.

PUBLICATIONS

For a full list of publications, visit my [Google Scholar Profile](#)