# Adrian Domínguez Castro, Ph.D.

AI & ML Engineer | LLMs & RAG Systems | AI for Science

Email       · Linkedin       · GitHub       · Google Scholar       Website

**Work Authorization: Permanent Resident (Green Card) / No sponsorship required**

## PROFESSIONAL SUMMARY:

Ph.D. in Physics and AI/ML Engineer specializing in agentic workflows and RAG systems for high-dimensional scientific data. Expert at architecting physics-informed ML models and production-ready systems to accelerate discovery in healthcare and computational chemistry.

## SELECTED EXPERIENCE

**Principal Data Scientist | AI/ML · Sept 2024-Present**
*ADC Scientific Consulting, USA.* — Independent consulting on AI/ML solutions for healthcare and scientific research

Selected engagements:

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

- Architected and deployed 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 publication. 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

**AI & ML:** Deep Learning, LLMs & RAG, Agentic Workflows (LangGraph), Statistical Modeling
**Computational Chemistry & Cheminformatics:** DFT, DFTB, Molecular Dynamics (MD), RDKit
**Systems & HPC:** Linux, High-Performance Computing, Automated Data Pipelines.
**Programming:** Python (NumPy, Pandas, PyTorch), C/C++, Shell.
**Leadership:** Cross-functional Leadership, Interdisciplinary Collaboration, Project Management

## PUBLICATIONS

**For a full list of publications, visit my** Google Scholar Profile