Adrian Domínguez Castro, Ph.D.

Data Scientist | Machine Learning | Computational Chemistry

Email · Linkedin · GitHub · Google Scholar · Website

SELECTED EXPERIENCE

Data Scientist | Machine Learning · Apr 2024-Present
ADC Scientific Consulting, USA. (Self-employed)

- Led a Wine Quality Prediction project using a Deep Neural Network, achieving 94.92% validation accuracy and highlighting key chemical features. Link

- Built an LSTM Autoencoder for anomaly detection in WTI crude oil prices, highlighting correlations with global crises and market shocks. Link

- Delivered end-to-end ML and cheminformatics pipelines (molecular descriptor generation, feature engineering, predictive modeling, deployment, visualization), producing actionable insights and client-ready reports accessible through my Portfolio

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.) · 2022 · University of Bremen, Germany

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

SKILLS

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

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.

PORTFOLIO HIGHLIGHTS – MACHINE LEARNING & DATA SCIENCE

Explore full projects on Portfolio

PUBLICATIONS

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