Adrian Domínguez Castro, Ph.D.

Machine Learning Engineer | Data Scientist

GitHub · Linkedin · Email

SELECTED EXPERIENCE

Machine Learning Engineer **Feb 2024-Present**
Freelance (Remote in USA)

- Designed, developed and optimized End-to-End Machine Learning and Data Science projects, showcasing them on GitHub (https://github.com/DrAdrianDC/Portfolio-for-Data-Science).
- Adapted and integrated state-of-the-art Machine Learning algorithms for predictive analysis in finance, computational chemistry and materials science, biomedical research, anomaly detection, image classification and clustering.
- Developed data science solutions using Python to automate preprocessing and data analysis, reducing a 90% of processing time.

Postdoctoral Research Scientist **Feb 2023-Jan 2024**
Vanderbilt University Nashville, TN, USA

- Designed, developed, and implemented Machine Learning projects, including deep learning models predicting physical-chemistry observables with over 85% accuracy, culminating in 1 publication.
- Led computational chemistry simulations and developed Python scripts to automate data collection, and data cleaning processes, reducing a 80% of processing time.

Doctoral Research Scientist **Oct 2018-Dec 2022**
University of Bremen Bremen, Germany

- Led all aspects of 3 multi-year research projects, resulting in 4 publications and developed data science solutions resulting in a 50% reduction of processing time.
- Managed data modeling efforts to develop advanced simulations and predictive models for computational chemistry, presenting insights in 10 + talks at scientific meetings. Built teams and forged collaborations across 5 countries (Germany, Spain, China, USA, France)
- Collaborated on the development of Deep Learning models for AI applications in Chemistry.

EDUCATION

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

B.Sc. in Radiochemistry · 2014 · InSTEC, Cuba

SKILLS

• Machine Learning • Deep Learning • Data Science • Statistical Analysis • Quantitative Analytics • Python Programming • Project Management • Communication

CERTIFICATIONS

- Machine Learning by Stanford University & DeepLearning.AI on Coursera.
- AI for Everyone by Stanford University & DeepLearning.AI on Coursera.
- Machine Learning Crash Course offered by Google

PORTFOLIO FOR MACHINE LEARNING AND DATA SCIENCE

Explore the projects in details at https://github.com/DrAdrianDC/Portfolio-for-Data-Science.

- **Project on Data Cleaning:** A comprehensive process of cleaning and preparing raw data for analysis and modeling.
  Tools & Techniques: Python, pandas, numpy, matplotlib, plotly, seaborn, scikit-learn
- **Breast Cancer Classification:** Classification problem using SVM) in biomedical research.
  Tools & Techniques: Python, ML, SVM, scikit-learn, numpy, pandas, matplotlib, seaborn

- **Wine Quality Prediction:** Predicting the quality of wines using physicochemical variables.
  Tools & Techniques: Python, ML, DL, XGBoost, Logistic regression, Random Forest, pandas, scikit-learn, tensorflow, keras, numpy, matplotlib, data visualization, Streamlit web app.
- **WTI Oil Prices Anomaly Detection:** Anomaly Detection in West Texas Intermediate (WTI) Crude Oil Prices.
  Tools & Techniques: Python, DL, yfinance, pandas, tensorflow, keras, numpy, matplotlib, data visualization, LSTM autoencoders
- **Apple Stock Market Prediction:** Apple stock market prediction using DL.
  Tools & Techniques: Python, yfinance, pandas,tensorflow, keras, numpy, matplotlib, data visualization, DL, LSTM
- **Image Classification:** Image Classification using Transfer Learning.
  Tools & Techniques: Python, ML, tensorflow, keras, seaborn, numpy, matplotlib, data visualization, DL, Transfer Learning,
- **DFT Meets Machine Learning:** Predicting hydrogen adsorption energies on rocksalt complex oxides combining DFT calculations and Machine Learning.
  Tools & Techniques: Python, ML, DL, Linear Regression, Random Forest, Neural networks, pandas, scikit-learn, tensorflow, keras, numpy, matplotlib
  Published in Theoretical Chemistry Accounts journal https://lnkd.in/ePBzVbsC
- **Clustering:** Clustering using the K-Means algorithm on the famous Iris dataset.
  Tools & Techniques: Python, ML, K-Means, pandas, numpy, matplotlib, seaborn, scikit-learn

PUBLICATIONS

[1] **Adrian Dominguez-Castro.** *DFT and machine learning for predicting hydrogen adsorption energies on rocksalt complex oxides.* **Theor Chem Acc 143, 50 (2024)** doi:10.1007/s00214-024-03124-x

[2] Michael Wagstaffe, **Adrian Dominguez-Castro**, Lukas Wenthaus, Steffen Palutke, Dmytro Kutnyakhov, Michael Heber, Federico Pressacco, Siarhei Dziarzhytski, Helena Gleißner, Verena Kristin Gupta, Harald Redlin, Adriel Dominguez, Thomas Frauenheim, Angel Rubio, Andreas Stierle, and Heshmat Noei. *Photoinduced Dynamics at the Water/TiO_2 (101) Interface.* **Phys. Rev. Lett.130, 108001 (2023)** doi:10.1103/PhysRevLett.130.108001

[3] **Adrian Domínguez-Castro** and Thomas Frauenheim. *Impact of vibronic coupling effects on light- driven charge transfer in pyrene-functionalized middle and large-sized metalloid gold nanoclusters from Ehrenfest dynamics.* **Phys. Chem. Chem. Phys., 2021, 23, 17129–17133** doi:10.1039/d1cp02890a

[4] **Adrian Domínguez-Castro**, Carlos R. Lien-Medrano, Khaoula Maghrebi, Sabri Messaoudi, Thomas Frauenheim and Arnaud Fihey. *Photoinduced charge-transfer in chromophore- labeled gold nanoclusters: quantum evidence of the critical role of ligands and vibronic couplings.* **Nanoscale, 2021, 13, 6786–6797** doi:10.1039/d1nr00213a

[5] Michael Wagstaffe, Lukas Wenthaus, **Adrian Dominguez-Castro**, Simon Chung, Guilherme Dalla Lana Semione, Steffen Palutke, Giuseppe Mercurio, Siarhei Dziarzhytski, Harald Redlin, Nicolai Klemke, Yudong Yang, Thomas Frauenheim, Adriel Dominguez, Franz Kärtner, Angel Rubio, Wilfried Wurth, Andreas Stierle, and Heshmat Noei. *Ultrafast Real-Time Dynamics of CO Oxidation over an Oxide Photocatalyst.* **ACS Catal. 2020, 10, 13650—13658** doi:10.1021/acscatal.0c04098

[6] **Adrian Domínguez-Castro**, Dariel Hernández, and Fernando Guzmán. *Insights into the interactions of biomolecules with small gold clusters: a theoretical study from a DFTB perspective.* **Theor. Chem. Acc. (2017) 136:84** doi:10.1007/s00214-017-2118-7

[7] **Adrian Dominguez-Castro**, Fernando Guzman, Yasser Novo-Fernandez. *Adsorption on a nanoporous organic polymer for clean energy applications: A multiscale modelling study using Density Functional Tight Binding Approach.* **Computational and Theoretical Chemistry 1102 (2017) 30–37** doi:10.1016/j.comptc.2016.12.037

[8] R. Castañeda-Arriaga, **A. Domínguez-Castro**, J. Lee, J. R Alvarez-Idaboy, N. Mora-Diez. *Chemical Repair of Protein Carbon-Centred Radicals: Long-Distance Dynamic Factors.* **Can. J. Chem., 2016, 94 (12): 1119-1126** doi:10.1139/cjc-2016-0230.