Adrian Domínguez-Castro, PhD

Machine Learning Engineer and Data Scientist

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WORK EXPERIENCE

Freelance Machine Learning Engineer and Data Scientist **Feb 2024-Present**
Remote (Based 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 biomedical research, chemistry and materials science, finance, anomaly detection, image classification and clustering.

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

- Designed, developed and implemented a Machine Learning model that predicts physical-chemistry observables with more than 85% accuracy, resulting in 1 publication.
- Led computational simulations and built and maintained data pipelines using Python for Machine Learning projects
- Used Python to automate data cleaning processes, saving 16 hours per week.

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

- Completed 3 multi-year research projects, resulting in 4 publications and improved data science solutions resulting in a 50% reduction in data acquisition and processing time.
- Led data modeling efforts to develop advanced simulations and predictive models for new nanoscience technologies, presenting insights at international scientific meetings. Built teams and forged collaborations across five countries (Germany, Spain, China, USA, France)
- Interpreted complex data sets, executed data analysis and visualization using Python.
- Assisted in developing Deep Learning models for AI in Chemistry with a 15% increased accuracy.

Graduate Research Fellow **Sept 2017-Jul 2018**
University of Groningen Groningen, The Netherlands

- Managed research on Theoretical Chemistry, and mentored junior team members. Optimized code for simulations and data science projects.
- Used Python to automate data analysis processes, reducing a 25% of processing time.

Visiting Research Scholar **Jan 2016-May 2016**
Thompson Rivers University Kamloops, Canada

- Developed computational modeling, and Data Science for Quantum Chemistry. Built teams and forged collaborations across two countries (Canada and Mexico), resulting in 1 publication.

Associate Junior Researcher **Sept 2015-Jul 2017**
Higher Institute for Technology and Applied Sciences (InSTEC) Havana, Cuba

- Led a team of 4 scientists to meet project milestones, optimizing computational modeling and developing advanced predictive models for Computational Chemistry, resulting in 2 publications
- Used Python to automate preprocessing and data analysis, reducing a 50% of processing time.

Assistant Professor **Sept 2014-Jul 2015**
Technological University of Havana (CUJAE) Havana, Cuba

- Delivered Lectures and Tutorials of Calculus, Differential Equations, and Numerical Mathematics (1st and 2nd years Electrical Engineering) And applied C/C++ Programming for Data Analysis, and Numerical Simulations.
- Mentored junior data analysts on machine learning techniques.

EDUCATION

Ph.D. (Dr. rer. nat.) **Oct 2018 - Dec 2022**
University of Bremen Bremen, Germany
Dissertation: Theoretical investigation on light- driven ultrafast dynamics in nanoscale
(Grade: magna cum laude)

B.Sc. Radiochemistry **Sept 2008 - Jun 2014**
Higher Institute for Technology and Applied Sciences (InSTEC) Havana, Cuba
Dissertation: Essential amino acids interacting with Fumonisin B1: A Theoretical Approach
(Grade: summa cum laude)

SKILLS

• Machine Learning • Deep Learning • Data Science • Statistical Analysis • Predictive Analytics • Problem-Solving • Project Management • Communication

Machine Learning Tools: TensorFlow, PyTorch, Keras, Scikit-learn
Programming Languages: Python, C/C++, SQL
Data Analysis & Visualization: Pandas, NumPy, Matplotlib, Seaborn, Streamlit

CERTIFICATIONS

- Machine Learning by Stanford University & DeepLearning.AI on Coursera.
- AI for Everyone by Stanford University & DeepLearning.AI on Coursera.

PROJECTS

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 Support Vector Machine (SVM) in biomedical research.
  Tools & Techniques: Python, Machine Learning, SVM, scikit-learn, numpy, pandas, matplotlib, seaborn
- **Wine Quality Prediction:** Predicting the quality of wines using physicochemical variables.
  Tools & Techniques: Python, Machine Learning, XGBoost, Logistic regression, Random Forest, Neural networks, 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, Deep Learning, yfinance, pandas, tensorflow, keras, numpy, matplotlib, data visualization, LSTM autoencoders
- **Apple Stock Market Prediction:** Apple stock market prediction using Deep Learning.
  Tools & Techniques: Python, yfinance, pandas,tensorflow, keras, numpy, matplotlib, data visualization, Deep Learning, LSTM
- **Image Classification:** Image Classification using Transfer Learning.
  Tools & Techniques: Python, Machine Learning, tensorflow, keras, seaborn, numpy, matplotlib, data visualization, Deep Learning, Transfer Learning,
- **DFT Meets Machine Learning:** Predicting hydrogen adsorption energies on rocksalt complex oxides combining DFT calculations and Machine Learning.
  Tools & Techniques: Python, Machine Learning, Deep Learning, 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, Machine Learning, 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.