

Adrian Domínguez-Castro, PhD

Data Scientist | Machine Learning | Data Analysis

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SUMMARY

Data Scientist with a PhD in Physics and 10 years of experience. Advanced knowledge in machine learning and statistical analysis. Skilled in Python and SQL. Proven track record of optimizing and implementing computational simulations and data-driven solutions for science and technology.

SKILLS

• Python • Machine Learning • Deep Learning • Data Science • SQL • Statistical Analysis

WORK EXPERIENCE

Postdoctoral Research Fellow

Feb 2023-Jan 2024

Vanderbilt University

Nashville, TN, USA

- Designed and implemented a machine learning system that predicts physical-chemistry observables with more than 85% accuracy.
- Managed simulations and data science projects related to experimental needs in Materials Science.

Doctoral Research Assistant

Oct 2018-Dec 2022

University of Bremen

Bremen, Germany

- Completed a multi-year research project, and improved data science solutions resulting in a 50% reduction in data acquisition and processing time.
- Optimized data modeling in developing advanced simulations and predictive models for new technologies in nanoscience, and communicated insights in international scientific meetings.
- Built teams and forged collaborations across five countries (Germany, Spain, China, USA, France)

Graduate Research Fellow

Sept 2017-Jul 2018

University of Groningen

Groningen, The Netherlands

- Managed research on Theoretical Chemistry, and mentored junior team members.

Visiting Research Scholar

Jan 2016-May 2016

Thompson Rivers University

Kamloops, Canada

- Developed computational modeling, data science and programming for Quantum Chemistry.
- Built teams and forged collaborations across two countries (Canada and Mexico)

Associate Junior Researcher

Sept 2015-Jul 2017

Higher Institute for Technology and Applied Sciences (InSTEC)

Havana, Cuba

- Led a team to meet project milestones and optimized computational modeling performance to automate preprocessing, reducing time taken by 50%.
- Developed and contributed to advanced predictive models for Computational Materials Science.

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)

EDUCATION

University of Bremen

Bremen, Germany

Ph.D. (Dr. rer. nat.)

Oct 2018 - Dec 2022

Dissertation: Theoretical investigation on light- driven ultrafast dynamics in nanoscale
(Grade: magna cum laude)

Higher Institute for Technology and Applied Sciences (InSTEC)

Havana, Cuba

B.Sc. Radiochemistry and Nuclear Chemistry

Sept 2008 - Jun 2014

Dissertation: Essential amino acids interacting with Fumonisin B1: A Theoretical Approach
(Grade: summa cum laude)

PORTFOLIO FOR DATA SCIENCE

Explore my data science projects in detail at <https://github.com/DrAdrianDC/Portfolio-for-Data-Science>.

CERTIFICATIONS

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

PUBLICATIONS

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](https://doi.org/10.1007/s00214-024-03124-x)

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/TiO₂ (101) Interface.

Phys. Rev. Lett.**130**, 108001 (2023) doi:[10.1103/PhysRevLett.130.108001](https://doi.org/10.1103/PhysRevLett.130.108001)

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](https://doi.org/10.1039/d1cp02890a)

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](https://doi.org/10.1039/d1nr00213a)

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](https://doi.org/10.1021/acscatal.0c04098)

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](https://doi.org/10.1007/s00214-017-2118-7)

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](https://doi.org/10.1016/j.comptc.2016.12.037)

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](https://doi.org/10.1139/cjc-2016-0230).