J. Fernando Fajardo-Rojas

Updated August 25, 2025

Ph.D. in Materials Science
Institute for Data Driven Dynamical Design – ID4
Department of Chemical and Biological Engineering
Colorado School of Mines
1500 Illinois St. Golden, CO, 80401
jfajardorojas@mines.edu — (+1) 720-854-5136

Research interests

My research interests lie at the intersection of machine learning and materials science. Specifically, I am interested in integrating data science, molecular simulation, and machine learning to understand and accelerate the discovery of functional materials for applications in energy, environmental sustainability, and health.

Education

Colorado School of Mines Golden, CO
PhD in Materials Science 2025
Advisor: Diego A. Gómez-Gualdrón
Thesis: *Data-Driven Development of Metal-Organic Frameworks: Synthesizability Insights and Thermodynamic Stability Predictions*

Universidad de los Andes Bogotá, Colonbia
PhD in Engineering 2021
Advisors: Diego Pradilla & Oscar Alvarez
Thesis: *Interfacial Behavior of Natural and Model Asphaltenes: A Multi-Scale Approach*

MS in Chemical Engineering 2021

Universidad Industrial de Santander Bucaramanga, Colombia
MS in Hydrocarbon Engineering 2016
BS in Chemical Engineering 2013

Honors & Awards

ID4 Excellece Award (Institute for Data Driven Dynamical Design - NSF) 2024
Granted to graduate students and/or postdocs who contribute significantly to ID4 intellectual merit, broader impacts and/or ID4 community building

Fulbright Scholarship "Colombian Doctoral Student" (Fulbright Colombia) 2018
Stipend and Travel Expenses

Doctoral Scholarship (Dept. of Chemical Eng., Universidad de los Andes) 2017
Tuition and Fees

Proposal & Grants

NSF Research Proposal – Award Abstract # 2450909 – CDS&E 2025
Transferable machine learning (ML) potentials to enable ML-based screening of adsorbents for separations involving chemisorption
PI: Diego A. Gómez-Gualdrón
Role: Contributor: *Involved in idea discussions that shaped the proposal content; responsible for developing visual aids.*

Publications

Complete list of publications in Google Scholar

1. Data-Driven Insights on the Impact of Functionalization on Metal–Organic Framework Free Energies
F. Fajardo-Rojas, R. Anderson, M. Li, R. Chang, D. A. Gómez-Gualdrón
*Chemistry of Materials (**2025**).* 10.1021/acs.chemmater.5c00129

2. MOFs to Enhance Green NH_3 Synthesis in Plasma Reactors: Hierarchical Computational Screening Enhanced by Iterative Machine Learning
T.W. Liu, **F. Fajardo-Rojas**, S. Addish, E. Martinez, D. A. Gómez-Gualdrón
*ACS Applied Materials & Interfaces (**2024**).* 10.1021/acsami.4c11396

3. Active learning of alchemical adsorption simulations: Towards a universal adsorption model
E. Osaro, **F. Fajardo-Rojas**, G. M. Cooper, D. A. Gómez-Gualdrón, Y. J. Colón
*Chemical Science (**2024**).* 10.1039/D4SC02156H

4. Framework-Topology-Controlled Singlet Fission in Metal-Organic Frameworks
S. Rajasree, J. Yu, **F. Fajardo-Rojas**, H. C. Fry, R. Anderson, X. Li, W. Xu, J. Duan, S. Goswami, K. Maindan, D.A. Gómez-Gualdrón, P. Deria
*JACS (**2023**).* 10.1021/jacs.3c03918

5. Theoretical Assessments of Pd-PdO phase transformation and its impacts on H_2O_2 synthesis and decomposition pathways
M. Vyas, **F. Fajardo-Rojas**, D.A. Gómez-Gualdrón, S. Kwon
*Catalysis Science & Technology (**2023**).* 10.1039/D3CY00404J

6. Deviation from Equilibrium Thermodynamics of an Asphaltene Model Compound During Compression-Expansion Experiments at Fluid-Fluid Interfaces
F. Fajardo-Rojas, O. Alvarez, J.R. Samaniuk, D. Pradilla
*Langmuir (**2021**).* 10.1021/acs.langmuir.0c03151

7. Probing Interfacial Structure and Dynamics of Model and Natural Asphaltenes at Fluid-Fluid Interfaces
F. Fajardo-Rojas, D. Pradilla, O. Alvarez, J.R. Samaniuk
*Langmuir (**2020**).* 10.1021/acs.langmuir.0c01320

Preprints

1. Highly Accurate and Fast Prediction of MOF Free Energy Via Machine Learning
A. Rubungo*, **F. Fajardo-Rojas***, D. A. Gómez-Gualdrón, A. Bousso Dieng. (**2025**).
* Equal contribution.
10.26434/chemrxiv-2025-93xmj

2. Interactions of Common Synthesis Solvents with MOFs Studied via Free Energies of Solvation: Implications on Stability and Polymorph Selection
F. Fajardo-Rojas, R. Anderson, K. Ardila, A. Pak, D. A. Gómez-Gualdrón. (**2025**).
10.26434/chemrxiv-2025-3phk2

3. Expert-Guided LLM Approach for Sequence-Aware Extraction of MOF Synthesis
X. Zhao, **F. Fajardo-Rojas**, J. Furst, K. Ardila, K. Langlois, Y. An, X Hu, F. Uribe-Romo, D. A. Gómez-Gualdrón, J. Greenberg. (**2025**).
10.26434/chemrxiv-2025-x90hc

Research experience

Colorado School of Mines Golden, CO
Research Assistant Fall 2021 – Summer 2025
Department of Chemical and Biological Engineering
Mentor: Diego A. Gómez-Gualdrón
Development of computational workflows (Machine Learning & Molecular Simulation) to assess thermodynamic stability of metal-organic frameworks (MOFs) and their performance in chemical separation. Physics-based representation of materials for machine learning.

Fulbright Scholar Fall 2018 – Summer 2019
Department of Chemical and Biological Engineering
Mentor: Joseph Samaniuk
Home Institution: Universidad de los Andes, Bogotá, Colombia
Linked the molecular-scale behavior of asphaltene molecules at fluid–fluid interfaces to the bulk stability and rheology of asphaltene-stabilized oil-water emulsions.

Universidad de los Andes Bogotá, Colombia
Research Project Specialist Spring 2021 - Summer 2021
Research Center, School of Engineering
Mentor: Diego Pradilla
Assessed the formulation of emulsion breakers for water–crude oil mixtures. Reported findings and proposed new directions to the sponsor company, Dow Chemical Colombia.

Research Assistant Spring 2017 - Spring 2018 & Fall 2019 – Spring 2021
Department of Chemical and Food Engineering
Mentors: Diego Pradilla & Oscar Alvarez
Integrated a multiscale approach to understand complex colloidal systems by combining interfacial microscopy and deformation studies with bulk rheology.

Teaching experience

Universidad Industrial de Santander Bucaramanga, Colombia

Lecturer, Department of Petroleum Engineering
Miscible Methods for Enhanced Oil Recovery – *Graduate Course* Fall 2020
Average student rating: 4.6/5.

Balance of Mass and Energy – *Undergraduate Course* Spring 2014 - Fall 2016
Transport Phenomena – *Undergraduate Course*
Thermodynamics – *Undergraduate Course*
Average student rating: Not available records.

Universidad de los Andes Bogotá, Colombia

Teaching Assistant, Department of Chemical Engineering
Intro. to Chemical Engineering – *Undergraduate Course* Spring 2017 - Spring 2021
Reaction Engineering – *Undergraduate Course*
Thermodynamics – *Undergraduate Course*
Average student rating: 4.7/5.
Main responsibilities: Lead the experimental section of the courses, and grading of the tests and projects.

Industry experience

Colombian Institute of Petroleum Floridablanca, Colombia
Universidad Industrial de Santander

Enhanced Oil Recovery Engineer Spring 2016 - Fall 2016
Main responsibilities: Led research on enhanced oil recovery (EOR) in Colombian oilfields, focusing on in-situ combustion and chemical flooding.

Talks and tutorials

Simulation-Free, Two-Dimensional Histograms as Effective Adsorbent Representations for Machine-Learning Based Adsorption Predictions
AIChE Annual Meeting, San Diego, CA Nov. 2024

Insights on the Synthesizability Likelihood of Metal-Organic Frameworks: Functionalization, Solvation, and Polymorphism
ACS Fall Meeting, Denver, CO Aug. 2024

Implications of Material Functionalization and Solvent Identity on the Synthesizability and Polymorph Selection of Metal-Organic Frameworks
AIChE Annual Meeting, Orlando, FL Nov. 2023

Probing Interfacial Structure and Dynamics of Asphaltenes and Model Asphaltenes at Fluid-Fluid Interfaces
AIChE Annual Meeting, Orlando, FL Nov. 2019

Mentoring

Colorado School of Mines Golden, Colorado

Materials Science REU Program
Luisa Ruiz, *currently PhD. student in Mat. Sci. & Eng. at Penn State* Summer. 2024
Vashti Trujillo, *currently BS. Mechatronics Eng. at CSU - Pueblo* Summer. 2023
Sumaya Adish, *currently PhD. student in Bio. Sci. at UNC - Chapel Hill* Summer. 2022

Summer Undergraduate Research Fellowship – SURF
Jack Canonico, *currently BS. Quantitative Biological Eng. at CSM* Summer. 2024

Secondary Advisor
Universidad de los Andes Bogotá, Colombia
Diego Ayala, *MS. Chemical Eng.*, currently Analyst at HINICIO 2023
Johana Pérez, *MS. Chemical Engineering*, currently R&D Scientist at DANEC 2021
Cesar Bucheli, *BS. Chemical Engineering*, currently Ph.D. at Brown University 2020

Reviewing & Service

Thesis Committee Member

Universidad Industrial de Santander Bucaramanga, Colombia
Sergio Castellanos, *MS. Petroleum Eng.* 2025
Bayron Torres, *MS. Petroleum Eng.* 2023

Universidad de los Andes Bogotá, Colombia
Mishel Porras, *MS. Chemical Eng.* 2023

Participation in Associations

Fulbright Program Colombia, *Selection Committee* 2022 -Present
Interdisciplinary Program Liaison, *Chemical Eng. Graduate Association (CEGA)* 2024

Journal Reviewing

Journal of Alloys and Compounds, Revista Facultad de Ingeniería Universidad de Antioquia, Revista Fuentes Universidad Industrial de Santander

Skills

Programming Language
Proficient in: Python, Bash, TensorFlow.
Familiar with: PyTorch, LaTeX.
Learning/Interested: JAX.

Molecular Simulation Software
LAMMPS, GROMACS.
Familir with: Quantum Espresso, Gaussian.

Other interests

Ultimate frisbee, climbing, cycling, running, soccer, coffee, photography.