JAIR FERNANDO FAJARDO-ROJAS

1613 Illinois St. Alderson Hall, Golden, CO 80401, USA

Email: fernando.fajardo.rojas@gmail.com| Phone: (+1) 720 854 5136 | Website: https://jfajardorojas.github.io/

Postdoctoral Fellow in Physics 2025 - Present

Colorado School of Mines, Advisor: Prof. Eric S. Toberer

Education

Ph.D. in Materials Science 2025

Colorado School of Mines, Advisor: Prof. Diego A. Gómez-Gualdrón

Ph.D. in Engineering 2021

Universidad de Los Andes, Advisor: Prof. Diego Pradilla & Prof. Oscar Alvarez

M.S. in Chemical Engineering 2021

Universidad de Los Andes

M.S. in Hydrocarbon Engineering 2016

Universidad Industrial de Santander

B.S. in Chemical Engineering 2013

Universidad Industrial de Santander

Honors & Awards

2024 Excellence Award by the Institute of Data-Driven Dynamics Design (ID4) - Colorado School of Mines

2024 Travel Award to attend "AI≡Science: Strengthening the Bond Between the Sciences and Artificial Intelligence" Workshop at University of California, Berkeley – Institute of Data-Driven Dynamics Design (ID4)

2018 Fulbright Scholar "Colombian Doctoral Student" – Fulbright Commission Colombia

Research Highlights

- Identified how functionalization influences the thermodynamic stability of metal-organic frameworks (MOFs) using data-driven analysis from data acquired via high-throughput molecular simulation.
- Developed a protocol that accelerates the calculations of solvation free energies in nanoporous materials via molecular simulation.
- Designed data-efficient strategies for training machine learning (ML) models to predict free energy and adsorption properties of MOFs.
- Co-developed representations of porous materials to enable ML prediction of adsorption properties and thermodynamic stability.

Proposal Contributions

- Transferable machine learning (ML) potentials to enable ML-based screening of adsorbents for separations involving chemisorption. Award amount: $320,117 – NSF funded
  Brainstorming, graphics, literature search, citation support

Peer-reviewed publications

11 publications, 5 as first or co-first author, * Equal contribution | Google Scholar

Under Review

(11) Machine Learning to Design Metal-Organic Frameworks: Progress and Challenges from a Data Efficiency Perspective. D. A. Gómez-Gualdrón, T.G. de Vilas, K. Ardila, **F. Fajardo-Rojas**, A. Pak. (Under Review in *Materials Horizons*)

(10) Highly Accurate and Fast Prediction of MOF Free Energy Via Machine Learning. A.N. Rubungo*, **F. Fajardo-Rojas***, D.A. Gómez-Gualdrón, A.B. Dieng. (*Pre-print* DOI: 10.26434/chemrxiv-2025-93xmj) (Under review in *JACS*)

(9) 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. (*Pre-print* DOI: 10.26434/chemrxiv-2025-3phk2) (Under Review in *Chemistry of Materials*)

Published or In Press

(8) 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. *Chem. Mater. 2025, 37, 15, 5502–5514.* DOI: 10.1021/acs.chemmater.5c00129

(7) MOFs to Enhance Green NH3 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 Appl. Mater. Interfaces 2024, 16, 49, 68506–68519.* DOI: 10.1021/acsami.4c11396

(6) 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. *Chem. Sci., 2024, 15, 17671-17684.* DOI: 10.1039/D4SC02156H

(5) Framework-Topology-Controlled Singlet Fission in Metal–Organic Frameworks. S.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. *J. Am. Chem. Soc. 2023, 145, 32, 17678–17688.* DOI: 10.1021/jacs.3c03918

(4) Novel Biosurfactants: Rationally Designed Surface-Active Peptides and In-Silico Evaluation at the Decane-Water Interface. J.V. Pérez-Bejarano, **F. Fajardo-Rojas**, O. Alvarez, J.C. Burgos, L.H. Reyes, D. Pradilla. *Process Biochem., 2023, 125, 84-95.* DOI: 10.1016/j.procbio.2022.11.012

(3) 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. *Catal. Sci. Technol., 2023, 13, 3828-3848.* DOI: 10.1039/D3CY00404J

(2) 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, 37, 5, 1799–1810*. DOI: 10.1021/acs.langmuir.0c03151

(1) 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, 36, 27, 7965–7979.* DOI: 10.1021/acs.langmuir.0c01320

In preparation

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. Pre-print, DOI: 10.26434/chemrxiv-2025-x90hc

Research Experience

Research Assistant 2021-2025
Department of Chemical and Biological Engineering | Colorado School of Mines
Supervisor: Diego A. Gómez-Gualdrón

Research Assistant 2017-2021
Department of Chemical and Food Engineering | Universidad de los Andes
Supervisor: Diego Pradilla

Researcher 2017-2015
Department of Petroleum Engineering | Universidad Industrial de Santander
Supervisor: Samuel Muñoz

Industry Experience

Project Specialist Summer 2021
Universidad de los Andes – Dow Chemical Colombia Bogotá, Colombia
Performance assessment of interfacially active formulations in destabilizing crude oil–water emulsions.

Enhanced Oil Recovery Engineer 2016
Colombian Institute of Petroleum – Universidad Industrial de Santander Bucaramanga, Colombia
Technical supervision of enhanced oil recovery (EOR) research and development in Colombia's petroleum fields.

Teaching Experience

Workshop instructor Fall 2022
Department of Petroleum Engineering - Universidad Industrial de Santander

Teaching Assistant 2017-2021
Department of Chemical and Food Engineering - Universidad de los Andes

Adjunct Faculty 2014–2016
Department of Petroleum Engineering - Universidad Industrial de Santander

Research Mentoring Experience

10 undergraduates mentored in different research experiences.

Research Experience for Undergraduates (REU) Summer Program, Colorado School of Mines

2025	Diego Hernandez	Currently: *Chemistry Student at Miami Dade College*
2025	Ruby Devaisher	Currently: *Physics & Math. Student at Coe College*
2024	Luisa Ruiz	Currently: *Ph.D. Student MatSci. & Eng. at Penn State University*
2023	Vashti Trujillo	Currently: *Mechatronics Student at Colorado State University-Pueblo*
2022	Sumaya Addish	Currently: *Ph.D. Student in Biological Science at UNC – Chapel Hill*

Summer Undergraduate Research Fellowship (SURF), Colorado School of Mines

2024	Jack Canonico	Currently: *Quantitative Biological Engineering Student at MINES*

Mines Undergraduate Research Fellowship (MURF), Colorado School of Mines

2025	Omar Mansurov	Currently: Chemical Eng. & Computer Science Student at MINES
2023	Enrique Martinez	Currently: Engineer at Chevron
2022	Dale Baum	
2022	Candan Erdemir	

Master Thesis Co-advisor

Universidad de los Andes, Bogotá, Colombia

2023	Diego Ayala	*M.S. Chemical Eng.*
2021	Johana Pérez	*M.S. Chemical Eng.*

Undergraduate Thesis Co-advisor

Universidad de los Andes, Bogotá, Colombia

2020	César Bucheli	*B.S. Chemical Eng.*

Universidad Industrial de Santander, Bucaramanga, Colombia

2017	Jadier Aristizabal & Daniela Mojica	*B.A. Petroleum Eng.*
2016	Andrés Vargas	*B.A. Petroleum Eng.*
2016	Jenifer Fierro & Lizet Rojas	*B.A. Petroleum Eng.*
2014	Clara Mendoza	*B.A. Chemical Eng.*
2014	Sebastian Quiceno & Julieth Vasquez	*B.A. Petroleum Eng.*

Oral Presentations

Conference Presentations

- *Coupled Human- and Machine Learning-Based Data-Driven Insights on the Impact of Functionalization on Metal-Organic Framework (MOF) Thermodynamic Stability.* AIChE Annual Meeting (2025). **Upcoming*
  F. Fajardo-Rojas, Mingwei Li, Remco Chang, Diego A. Gómez-Gualdrón.

- *Simulation-Free, Two-Dimensional Histograms as Effective Adsorbent Representations for Machine-Learning Based Adsorption Predictions.* AIChE Annual Meeting (2024).
  F. Fajardo-Rojas, T.W. Liu, T. Gercina de Vilas, D.A. Gómez-Gualdrón.
- *Insights on the Synthesizability likelihood of Metal-Organic Frameworks: Functionalization, solvation, and polymorphism.* ACS Fall Meeting (2024).
  F. Fajardo-Rojas, R. Anderson, D.A. Gómez-Gualdrón.
- *Implications of Material Functionalization and Solvent Identity on the Synthesizability and Polymorph Selection of Metal-Organic Frameworks.* AIChE Annual Meeting (2023).
  F. Fajardo-Rojas, R. Anderson, D.A. Gómez-Gualdrón.
- *Probing Interfacial Structure and Dynamics of Asphaltenes and Model Asphaltenes at Fluid-Fluid Interfaces*. AIChE Annual Meeting (2019).
  F. Fajardo-Rojas, D. Pradilla, O. Alvarez, J. Samaniuk.

Poster Presentations

- *From Data to Discovery: Developing Data-Efficient Frameworks to Enable the Discovery of Porous Materials.* AIChE Annual Meeting (2025).**Upcoming*
  F. Fajardo-Rojas. Meet the Faculty and Post-Doc Candidates Poster Session.
- *Accelerating the Design Cycle of Materials for Energy Applications: Harnessing Data to Bridge the Gap between Prototypes and Synthesis*. AIChE Annual Meeting (2024).
  F. Fajardo-Rojas. Meet the Faculty and Post-Doc Candidates Poster Session.

Service

Reviewing

Conference Reviewing

2023 - present	Symposium on Hydrocarbons Research, Universidad Industrial de Santander, Colombia

Journal Reviewing

2025 - present	Scientific Reports
2025 - present	Journal of Alloys and Compounds
2020 - present	Journal of School of Engineering Universidad de Antioquia (REDIN), Colombia

Outreach

Fulbright Commission Colombia

2022 - present	Fulbright Scholarship Review and Selection Committee

Leadership

Colorado School of Mines

2024	CEGA – Chemical Engineering Graduate Association – *Interdisciplinary Programs Liaison*
2022	GSG – Graduate Students Government – *Materials Science Representative*

Society of Petroleum Engineers, SPE

2017-2019	Universidad de los Andes, Student Chapter - *President*

References

Prof. Eric S. Toberer
Professor
Physics
Materials Science Program Director
Colorado School of Mines
etoberer@mines.edu

Prof. Diego A. Gómez-Gualdrón
Associate Professor
Chemical and Biological Engineering
Colorado School of Mines
dgomezgualdron@mines.edu

Prof. Alexander J. Pak
Assistant Professor
Chemical and Biological Engineering
Colorado School of Mines
samaniuk@mines.edu