JAIR FERNANDO FAJARDO-ROJAS

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Postdoctoral Fellow in Physics, *Colorado School of Mines* 2025 - Present
Advisor: Prof. Eric S. Toberer

Education

Ph.D. in Materials Science, *Colorado School of Mines* 2025
Advisor: Prof. Diego A. Gómez-Gualdrón

Ph.D. in Engineering (Chemical Engineering), *Universidad de Los Andes, Colombia* 2021
Advisor: Prof. Diego Pradilla & Prof. Oscar Alvarez

M.S. in Chemical Engineering, *Universidad de Los Andes, Colombia* 2021

M.S. in Hydrocarbon Engineering, *Universidad Industrial de Santander, Colombia* 2016

B.S. in Chemical Engineering, *Universidad Industrial de Santander, Colombia* 2013

Honors & Awards

2024 Excellence Award by the Institute of Data-Driven Dynamics Design (ID4) - NSF (*For academic and community contributions within the institute*)

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

2018 Fulbright Scholar "Colombian Doctoral Student" – Fulbright Commission Colombia (*Travel & Stipend)*

Research Highlights

- Revealed functionalization role in MOF thermodynamic stability via high-throughput simulation and data-driven analysis.
- Developed a protocol to accelerate free energy of solvation calculation via molecular simulation in nanoporous materials.
- Designed data-efficient machine learning (ML) strategies to predict MOF free energy and adsorption properties.
- Co-developed material representations enabling ML predictions of porous materials adsorption properties and stability.

Proposals

- Transferable machine learning (ML) potentials to enable ML-based screening of adsorbents for separations involving chemisorption. Award amount: $320,117 – NSF funded (Aug. 2025)
  Contributor: Brainstorming, graphics, literature search, citation support
- Generative design of thermodynamically stable metal-organic frameworks via symmetry-aware diffusion models. Computational award: 200,000 core-hour credits – NSF-ACCESS granted (Oct. 2025).
  Principal investigator

Peer-reviewed publications

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

Published

(11) †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. *Chem. Mater. 2026, 38, 2, 607–618*. DOI: 10.1021/acs.chemmater.5c01410

(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. *J. Am. Chem. Soc. 2025, 147, 52, 48035–48045.* DOI: 10.1021/jacs.5c13960

(9) 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. *Mater. Horiz.*, 2026, Advance Article. DOI: 10.1039/D5MH01467K

(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

Preprints

- 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

Postdoctoral Fellow 2025-present

Department of Physics, *Colorado School of Mines,* Supervisor: Eric S. Toberer

Building AI-enabled, multiscale computational workflows for predictive materials design, emphasizing integration between simulation, data-driven learning, and experimentation.

Research Assistant 2021-2025

Department of Chemical and Biological Engineering, *Colorado School of Mines,* Supervisor: Diego A. Gómez-Gualdrón

Developed computational frameworks to accelerate data-driven analysis and machine learning-based prediction of adsorption and thermodynamic stability in porous materials.

Research Assistant 2017-2021

Department of Chemical and Food Engineering, *Universidad de los Andes, Colombia,* Supervisor: Diego Pradilla

Conducted experiments to elucidate multi-scale structure–property relationships governing the behavior of surface-active molecules at fluid–fluid interfaces for colloidal systems design.

Researcher 2017-2015

Department of Petroleum Engineering, *Universidad Industrial de Santander, Colombia,* Supervisor: Samuel Muñoz

Evaluated combustion reaction kinetics under oil reservoir conditions to assess how oil composition and reservoir heterogeneity affect in-situ combustion performance for enhanced oil recovery.

Collaborations with Industry

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

Enhanced oil recovery via miscible methods

Teaching Assistant 2017-2021

Department of Chemical and Food Engineering - Universidad de los Andes

Introduction to Chemical Engineering, Thermodynamics, Reaction Kinetics

Adjunct Faculty 2014–2016

Department of Petroleum Engineering - Universidad Industrial de Santander

Thermodynamics, Transport Phenomena

Research Mentoring Experience

10 undergraduate students mentored through 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	

Eight theses co-advised in different graduate and undergraduate programs.

Master Thesis Co-advisor

Universidad de los Andes, Colombia

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

Undergraduate Thesis Co-advisor

Universidad de los Andes, Colombia

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

Universidad Industrial de Santander, 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

Invited Talks

- *Highly Accurate and Fast Prediction of MOF Free Energy Via Machine Learning.* NSF Institute for Data-Driven Dynamics Design (ID4). ID4 Fall meeting, Golden, Colorado (Oct. 2025).
  F. Fajardo-Rojas, A. N. Rubungo, A. B. Dieng, D. A. Gómez-Gualdrón.

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, Boston, Massachusetts (Nov. 2025). **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, San Diego, California, (Nov. 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, Denver, Colorado (Aug. 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, Orlando, Florida (Nov. 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, Orlando, Florida (Nov. 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, Boston, Massachusetts (Nov. 2025). **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, San Diego, California (Nov. 2024). **F. Fajardo-Rojas.** Meet the Faculty and Post-Doc Candidates Poster Session.

Service

Reviewing

Conference Reviewing

Symposium on Hydrocarbons Research, *Universidad Industrial de Santander, Colombia*

Journal Reviewing

Scientific Reports, Journal of Alloys and Compounds

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*