

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, <i>Colorado School of Mines</i>	2025
Advisor: Prof. Diego A. Gómez-Gualdrón	
Ph.D. in Engineering (Chemical Engineering), <i>Universidad de Los Andes, Colombia</i>	2021
Advisor: Prof. Diego Pradilla & Prof. Oscar Alvarez	
M.S. in Chemical Engineering, <i>Universidad de Los Andes, Colombia</i>	2021
M.S. in Hydrocarbon Engineering, <i>Universidad Industrial de Santander, Colombia</i>	2016
B.S. in Chemical Engineering, <i>Universidad Industrial de Santander, Colombia</i>	2013

Honors & Awards

2024	Excellence Award by the Institute of Data-Driven Dynamics Design (ID4) - NSF (<i>For academic and community contributions within the institute</i>)
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 (<i>Travel & Stipend</i>)

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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1016/j.procbio.2022.11.012)
- (3) Theoretical Assessments of Pd–PdO Phase Transformation and Its Impacts on H₂O₂ 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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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 Canonicco 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*

References

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Chemical and Biological Engineering
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Prof. Nanette Boyle
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