

JAIR FERNANDO FAJARDO-ROJAS

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Postdoctoral Fellow in Physics, *Colorado School of Mines*

2025 - Present

Advisor: Prof. Eric S. Toberer

Education

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| Ph.D. in Materials Science, <i>Colorado School of Mines</i> | 2025 |
| <i>Advisor: Prof. Diego A. Gómez-Gualdrón</i> | |
| Ph.D. in Engineering (Chemical Engineering), <i>Universidad de Los Andes, Colombia</i> | 2021 |
| <i>Advisor: Prof. Diego Pradilla & Prof. Oscar Alvarez</i> | |
| 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

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| 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

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| Postdoctoral Fellow | 2025-present |
| Department of Physics, <i>Colorado School of Mines</i> , Supervisor: Eric S. Toberer <i>Building AI-enabled, multiscale computational workflows for predictive materials design, emphasizing integration between simulation, data-driven learning, and experimentation.</i> | |
| Research Assistant | 2021–2025 |
| Department of Chemical and Biological Engineering, <i>Colorado School of Mines</i> , Supervisor: Diego A. Gómez-Gualdrón <i>Developed computational frameworks to accelerate data-driven analysis and machine learning-based prediction of adsorption and thermodynamic stability in porous materials.</i> | |
| Research Assistant | 2017–2021 |
| Department of Chemical and Food Engineering, <i>Universidad de los Andes, Colombia</i> , Supervisor: Diego Pradilla <i>Conducted experiments to elucidate multi-scale structure–property relationships governing the behavior of surface-active molecules at fluid–fluid interfaces for colloidal systems design.</i> | |
| Researcher | 2017–2015 |
| Department of Petroleum Engineering, <i>Universidad Industrial de Santander, Colombia</i> , Supervisor: Samuel Muñoz <i>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.</i> | |

Collaborations with Industry

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| Project Specialist | Summer 2021 |
| Universidad de los Andes – Dow Chemical Colombia Bogotá, Colombia <i>Performance assessment of interfacially active formulations in destabilizing crude oil–water emulsions.</i> | |
| Enhanced Oil Recovery Engineer | 2016 |
| Colombian Institute of Petroleum – Universidad Industrial de Santander Bucaramanga, Colombia <i>Technical supervision of enhanced oil recovery (EOR) research and development in Colombia's petroleum fields.</i> | |

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

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

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

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| 2024 | Jack Canonico | Currently: <i>Quantitative Biological Engineering Student at MINES</i> |
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Mines Undergraduate Research Fellowship (MURF), Colorado School of Mines

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| 2025 | Omar Mansurov | Currently: <i>Chemical Eng. & Computer Science Student at MINES</i> |
| 2023 | Enrique Martinez | Currently: <i>Engineer at Chevron</i> |
| 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

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| 2023 | Diego Ayala | <i>M.S. Chemical Eng.</i> |
| 2021 | Johana Pérez | <i>M.S. Chemical Eng.</i> |

Undergraduate Thesis Co-advisor

Universidad de los Andes, Colombia

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| 2020 | César Bucheli | <i>B.S. Chemical Eng.</i> |
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Universidad Industrial de Santander, Colombia

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

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

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

Prof. Nanette Boyle
Dept. Head & Associate Professor
Chemical and Biological Engineering
Colorado School of Mines
nboyle@mines.edu