

Jacques Esterhuizen

MACHINE LEARNING SCIENTIST

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Education

Ph.D. Chemical Engineering, GPA:3.97

UNIVERSITY OF MICHIGAN

Sept. 2017 - Sept. 2022

Ann Arbor, Michigan

M.S.E. Chemical Engineering, GPA:3.96

UNIVERSITY OF MICHIGAN

Sept. 2017 - May 2020

Ann Arbor, Michigan

B.S. Chemical Engineering, *Magna Cum Laude*, GPA:3.82

UNIVERSITY OF SOUTHERN CALIFORNIA

Aug. 2013 - May 2017

Los Angeles, California

Experience

Applied Scientist II

AMAZON WEB SERVICES

Sept. 2022–Present

San Francisco, California

Graduate Research Assistant

UNIVERSITY OF MICHIGAN

Sept. 2017–Sept. 2022

Ann Arbor, Michigan

Undergraduate Research Assistant

UNIVERSITY OF SOUTHERN CALIFORNIA

May 2016–May 2017

Los Angeles, California

Honors & Awards

Richard F. and Eleanor A. Towner Prize for Distinguished Academic Achievement in Chemical Engineering

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

January 2022

- College of engineering award presented to the outstanding Ph.D. students in each degree program. Criteria considered by the Chemical Engineering department awards committee included active participation in leadership, service to the department, and academic and research performance.

Department of Chemical Engineering Excellence in Research Award

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

September 2021

- Annual award to recognize outstanding research contributions in Chemical Engineering.

2nd Place Oral Presentation at Chemical Engineering Graduate Student Research Symposium

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

September 2021

Catalysis and Reaction Engineering Division Travel Award

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

San Francisco, California

November 2020

J. Robert Beyster Computational Innovation Graduate Fellowship

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

September 2020

- College of engineering fellowship to support cutting-edge research in a variety of fields linking high performance computing, networking, and storage to applications of societal importance.

1st Place at Michigan Data Science Team's MDatahack

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

January 2019

Distinction on Doctoral Candidacy Exam

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

May 2018

- Honor reserved for the best student (academics and research) in the first-year chemical engineering PhD class.

Rackham Graduate Student Research Grant

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

March 2018

USC Provost's Undergraduate Research Fellowship

UNIVERSITY OF SOUTHERN CALIFORNIA

Los Angeles, California

May 2016–May 2017

Publications

1. Jacques A. Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Interpretable machine learning for knowledge generation in heterogeneous catalysis. *Nature Catalysis*, pages 1–10, March 2022. Publisher: Nature Publishing Group
2. Jacques A. Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Uncovering Electronic and Geometric Descriptors of Chemical Activity for Metal Alloys and Oxides Using Unsupervised Machine Learning. *Chem Catalysis*, 1:1–18, August 2021
 - Spotlighted in *Trends in Chemistry*: Noushin Omidvar and Hongliang Xin. Algorithm-derived feature representations for explainable AI in catalysis. *Trends in Chemistry*, October 2021
3. Jacques A. Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Theory-Guided Machine Learning Finds Geometric Structure-Property Relationships for Chemisorption on Subsurface Alloys. *Chem*, 6(11):3100–3117, November 2020
4. Nicholas M. Orchanian, Lorena E. Hong, John A. Skrainka, Jacques A. Esterhuizen, Damir A. Popov, and Smaranda C. Marinescu. Surface-Immobilized Conjugated Polymers Incorporating Rhenium Bipyridine Motifs for Electrocatalytic and Photocatalytic CO₂ Reduction. *ACS Applied Energy Materials*, 2(1):110–123, January 2019
5. Bryan R. Goldsmith, Jacques Esterhuizen, Jin-Xun Liu, Christopher J. Bartel, and Christopher Sutton. Machine Learning for Heterogeneous Catalyst Design and Discovery. *AIChE Journal*, 64(7):2311–2323, July 2018

Presentations

1. Jacques Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Unsupervised Machine Learning to Extract the Electronic and Chemical Properties of Alloy and Metal Oxide Surfaces. AIChE Annual Meeting, November 2021, Oral Presentation
2. Jacques Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Machine-learning Interpretable Chemisorption Models for Alloys. Michigan Catalysis Society Symposium, September 2021, Oral Presentation
3. Jacques Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Unsupervised Learning of Electronic-structure Descriptors for Alloy and Metal Oxide Surfaces. ACS Fall Meeting, August 2021, Oral Presentation
4. , Oral Presentation
5. Jacques Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Intelligible Machine Learning Models for Chemisorption on Alloys: Finding Predictive Geometric Structure-Property Relationships. ACS Spring Meeting, April 2021, Oral Presentation
6. Jacques Esterhuizen, Bryan R. Goldsmith, and Suljo Linic. Theory-Guided, Interpretable Machine Learning Finds Predictive Geometric Structure-Property Relationships for Chemisorption on Alloys. AIChE Annual Meeting, November 2020, Oral Presentation

Skills

Machine learning	Regression, classification, unsupervised learning, interpretable machine learning algorithms, active learning, Bayesian global optimization, deep learning, transformers, information retrieval, agents
Applied mathematics	Multivariate calculus, differential equation modeling, applied numerical methods, optimization, statistics, probability, linear algebra, signal processing
Computer programming	Python (with expert-level proficiency in scientific and numerical packages including NumPy, SciPy, Matplotlib, Scikit-Learn, and PyTorch), Matlab, linux/unix, LaTeX, Julia
Chemical engineering	Statistical mechanics, reaction kinetics, fluid mechanics, heat transport, mass transport
Computational chemistry	VASP, Pymatgen, ASE, cheminformatics

Service

Recruitment Chair

March 2019

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

- One of three chairs who organized and hosted the chemical engineering departmental recruitment weekend for visiting admitted students. Recruited a class of 27 first year students.
- Optimized recruitment weekend visit planning for future years by implementing a simulated annealing Monte Carlo algorithm for automatically scheduling faculty meetings with visiting students.

Peer reviewer

December 2021–present

ACS CATALYSIS (2), ACS ENERGY LETTERS (1)

Teaching

Graduate Student Instructor

January 2020–May 2020

UNIVERSITY OF MICHIGAN

Ann Arbor, Michigan

- CHE528: Graduate Chemical Reaction Engineering (Winter 2020)