Joshua L. Lansford

PHD CANDIDATE IN CHEMICAL ENGINEERING · UNIVERSITY OF DELAWARE

☐ +1 (703)-400-3046 | ☑ lansford@udel.edu | ☑ JLans | ☐ jlansford | ☎ Joshua L. Lansford

Education

University of Delaware, College of Engineering

Newark, DE

Major: PhD Candidate in Chemical Engineering, GPA: 3.8

2015 - 2020 (Expected)

Advisor: Dr. Dionisios G. Vlachos

University of Virginia, School of Engineering and Applied Science

Charlottesville, VA

Major: B.S. in Chemical Engineering with High Distinction and a minor in Engineering Business, GPA: 3.8

2009 - 2013

Interests and Skills

Research Areas: machine learning, uncertainty quantification, electrocatalysis, fuel cells, and batteries

- Machine learning and uncertainty quantification of stochastic and deterministic models
- Applications in characterization and micro-kinetic modeling using transition state theories and statistical mechanics, including: heterogeneous catalysis, spectroscopy, surface science, and quantum chemistry

Programming Languages: Python, Unix, SAS, SQL, Aspen, MATLAB, Tableau, Java, JavaScript, VBA, HTML, Mathcad

- Contributor to open source atomic simulation python software ASE
- Built the University of Delaware's Proxify bookmark into a Chrome Extension

Certifications: Machine Learning by Stanford University, Neural Networks and Deep Learning by Deeplearning.Al (Coursera)

Honors and Awards

2019-2020 - Blue Waters Graduate Fellowship, first place at the AICHE poster completion in the CRE Division (co-author)

- **2019** Catalysis Club of Philadelphia (CCP) Ted Koch Travel Award, Deep Learning for Science School at Berkeley Travel Grant, Kokes Award for the 26th North American Catalysis Society (NACS) Conference
- **2018** Phillip and Ruth Evans Fellowship, University of Delaware Professional Education Development Award, ISCRE25 Graduate Student Travel Grant, CRE Division AlChE Graduate Student Travel Grant
- 2017 National Science Foundation Graduate Research Fellowship, Honorable Mention
- 2013 Louis T. Rader Chemical Engineering Prize, Awarded first place by Bill Clinton on Up to Us fiscal policy campaign
- **2012** Second place at the AICHE student poster competition (presenter)

Pre-2012 - Donald and Jean Heim, Dr. John Kenneth Haviland, and ExxonMobil Teagle Scholarships

Research Experience

University of Delaware - Advisor: Prof. Dionisios G. Vlachos

Newark, DE

Topic Combined Physics- and Data-based Model Development with Uncertainty Quantification for Catalyst Characterization and Kinetic Modeling

2015 - Current

- Developed theory to explain vibrational scaling of chemisorbates on transition metal surfaces from quantum principles
- Enforced physical constraints in design of a neural network that performs multinomial regression for structure prediction from spectra using two-levels of synthetic data and a closed-form derivation of the Wasserstein loss with respect to the softmax
- Quantified uncertainty in a multi-scale oxygen reduction kinetic model using probabilistic graphical modeling (PGM)

University of Connecticut

Storrs, CT

2012

National Science Foundation Research Fellowship

 Developed predictive fluid catalytic cracking model that split effects of the support matrix and active zeolite catalyst to better determine gasoil conversion and product yields

University of Virginia Organic Synthesis Lab

Charlottesville, VA

Determined optimal reaction conditions for stereospecific mechanisms

2010

Teaching & Research Advising

University of Delaware	Newark, DE
Graduate Student Mentor – Scaling of frequencies and entropies across surfaces	2019 – Current
Graduate Student Mentor – Characterizing bimetallics using computational infrared spectroscopy and phase diagrams	Current
Undergraduate Mentor – Combining infrared and X-ray absorption spectra for structure generation via genetic algorithms	2019 – Current
Undergraduate Mentor – CO oxidation descriptor selection with partial least squares	2017 - 2019
Teaching Assistant – Process design	Spring, 2017

Journal Publications

J. L. Lansford and D. G. Vlachos, Infrared Spectroscopy Data- and Physics-driven Machine Learning for Characterizing Surface Microstructure of Complex Materials. Nat. Commun. 11, 1513 (2020)

Initiated, designed, and taught a new in-person team-building class for honors students

- M. Núñez, J. L. Lansford, and D.G. Vlachos, Optimization of the facet structure of transition-metal catalysts applied to the oxygen reduction reaction. Nat. Chem. 11, 449–456 (2019).
- J. Feng, J. L. Lansford, A. Mironenko, D. B. Pourkargar, D. G. Vlachos, M. A. Katsoulakis, Non-parametric correlative uncertainty quantification and sensitivity analysis: Application to a Langmuir bimolecular adsorption model. AIP Adv. 8, 035021 (2018).
- J. L. Lansford, A. V. Mironenko, and D. G. Vlachos, Scaling relationships and theory for vibrational frequencies of adsorbates on transition metal surfaces. Nat. Commun. 8, No. 1842 (2017).
- J. Feng*, J. L. Lansford*, M. A. Katsoulakis, and D. G. Vlachos, Combining Uncertain Data and Expert Knowledge with Physics-Based Graphical Models for Quantifying Model Uncertainty (submitted) *contributed equally to this work
- J. L. Lansford*, N. R. Quiroz*, and D. G. Vlachos, Agile Software for Rapid Product Quantification under Uncertainty using Principal Component Regression of Infrared Spectra with Analysis through Deconvolution (submitted) *contributed equally to this work
- J. L. Lansford and D. G. Vlachos, Electron Density-Based Machine Learning for Accelerating Quantum Calculations (In Preparation)
- J. L. Lansford and D. G. Vlachos, Optimal Probe Molecule Selection for Characterizing Surface Microstructure: a combined physics- and data-based approach (In Preparation)
- J. L. Lansford, Sophia Kurdziel, and D. G. Vlachos, Theory and Scaling for Brønsted Evans –Polanyi Energy and Frequency Relationships on Surfaces (In Preparation)
- N. R. Quiroz, J. L. Lansford, and D. G. Vlachos, Coupling Experimental Kinetics and Thermodynamic Modeling with UV-Vis for Fundamental Studies and Speciation Quantification (In Preparation)

Invited Talks. Presentations and Posters

The Center for Dynamics and Control of Materials – Invited Talk (Josh Lansford)	Austin, TX
Infrared Spectroscopy Data- and Physics-driven Machine Learning for Characterizing Complex Surface Structure	e Feb. 2020
AIChE Meeting Presentation	Orlando, FL
Computational Modeling of operando Infrared Spectroscopy for Site-Specific Catalyst Characterization	Nov. 2019
North American Catalysis Society Meeting Presentation	Chicago, IL
Catalyst Site Characterization from Complex Infrared Spectroscopy	June 2019
Blue Waters Symposium Presentation	Sunriver, OR
Electron Density-Based Machine Learning for Accelerating Quantum Calculations	June 2019

Joshua Lansford – Curriculum Vitae	2020-05-15
Catalysis Club of Philadelphia Poster Competition	Philadelphia, PA
Forward and Inverse Modeling for Catalyst Characterization from Complex Vibrational Spectroscopy	Nov. 2018
AIChE Meeting Presentation	Pittsburgh, PA
Catalyst Characterization from Complex Infrared Spectroscopy: A Machine Learning Approach	Oct. 2018
Gordon Research Conference Poster Presentation	New London, NH
Entropic Effects on Microkinetic Modeling	June 2018
International Symposia of Chemical Reaction Engineering (ISCRE25) - Invited Talk (Dion Vlachos)	Florence, Italy
Catalyst Structure Prediction via DFT, Theory, and Machine Learning	May 2018
Catalysis Club of Philadelphia Poster Competition	Philadelphia, PA
Scaling Relations for Adsorbate Vibrations on Transition Metal Surfaces	Nov. 2017
AIChE Meeting Presentation	Minneapolis, MN
Adsorbate Vibrations on Transition Metal Surfaces: Applications and Theory	Oct. 2017
AIChE Student Poster Competition	Pittsburgh, PA
Separation of Catalyst Kinetics for Maximizing Gasoline Output, Yield, and Selectivity	Oct. 2012
In decades Manual Francisco	
Industry Work Experience Capital One Bank	Mal oon V/A
Senior Data Analyst: National Expansion	McLean, VA 2014 -2015
Developed geocoding system to map customer ATM transactions at foreign-owned ATMs	2014 2010
 Created Tableau tool that provides daily updates to 10 Capital One Cafes 	
 Converted organization's data library to Tableau infrastructure and scaled to all markets of interest 	est
Data Analyst: Bank Operations	2013 -2014
 Led self-proposed initiative to automate case tracking system for five business teams. Headed t 	wo IT
teams and coordinated with business teams in addition to developing and mapping out the auto	mated
system – saved 25-50 business hours per day	
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Service & Leadership, Professional Affiliations Reviewer	
The Journal of Physical Chemistry	
Memberships	
American Institute of Chemical Engineers (AICHE), Catalysis Club of Philadelphia (CCP)	
Harvard University	Cambridge, MA
Undergraduate Resident Tutor: Leverett House	2019 – Current
 Live with and advise Harvard undergrads on research and graduate school 	
University of Virginia	Charlottesville, VA
University Dormitory Resident Advisor	2010 – 2013
Live with and advise freshmen on transition from high school to college	
President of UVA OXE Chemical Engineering Honor Society	0040 0040
	2012 – 2013
 Organized tutoring, research panels, and other service and leadership opportunities 	
	2012 - 2013 2012 - 2013