# Joshua L. Lansford

PhD Candidate In Chemical Engineering · University of Delaware
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## Education

**University of Delaware, College of Engineering** *Newark, DE*
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*
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.AI (Coursera)

## Honors and Awards

**2019-2020** – Blue Waters Graduate Fellowship

**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, first place at the AICHE poster completion in the CRE Division (co-author)

**2018** – Phillip and Ruth Evans Fellowship, University of Delaware Professional Education Development Award, ISCRE25 Graduate Student Travel Grant, CRE Division AIChE 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

## 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*

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

## 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)

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 *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*

**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*

## Research Experience

**University of Delaware** *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*

National Science Foundation Undergraduate Research Fellowship *2012*

- 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*

## Industry Work Experience

**Capital One Bank** *McLean, VA*

Senior Data Analyst: National Expansion *2014 –2015*

- Developed geocoding system to map customer ATM transactions at foreign-owned ATMs
- 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.

Data Analyst: Bank Operations *2013 –2014*

- Led self-proposed initiative to automate case tracking system for five business teams. Headed two IT teams and coordinated with business teams in addition to developing and mapping out the automated system – saved 25-50 business hours per day

## Service, Leadership, and 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 *2012 – 2013*

- Organized tutoring, research panels, and other service and leadership opportunities

Co-President of UVA Wahoo Wizards Educational Outreach Group *2012 – 2013*

- Developed and led new science experiments for low-income elementary school students