Joshua L. Lansford

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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: Chemical Engineering with High Distinction and a minor in Engineering Business, GPA: 3.8	2009 – 2013

Interests and Skills

Research Areas: 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: includes 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, see Github for personal projects and documentation.
- Developed the University of Delaware's Proxify bookmark into a Chrome Extension for downloading scientific journals

Honors and Awards

- 2019-2020 – Blue Waters Graduate Fellowship
- 2019 – Catalysis Club of Philadelphia (CCP) Ted Koch Travel Award
- 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, First place national winner of the Up to Us National Debt Campaign
- 2012 – Second place at the AICHE student poster competition
- Scholarships: 2011 – Donald and Jean Heim, 2010 – Dr. John Kenneth Haviland, 2009 – ExxonMobil Teagle

Research Experience

University of Delaware – Advisor: Dr. 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**
National Science Foundation 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 and ran ion-exchange separations	2010

Teaching & Research Advising

University of Delaware	**Newark, DE**
Undergraduate Mentor – Combining infrared and X-ray absorption spectra for structure generation via genetic algorithms	2019
Undergraduate Thesis Mentor – CO oxidation descriptor selection with partial least squares	2017 – 2019
REU Mentor – Feature selection for rapid catalyst screening with principle component analysis	Summer, 2017
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, Generating synthetic IR spectra to reconstruct local catalyst microstructure from DFT, theory, and machine learning. Nat. Commun. (under revision)

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. (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. L. Lansford and D. G. Vlachos, Electron Density-Based Machine Learning for Accelerating Quantum Calculations (In Preparation)

J. L. Lansford, J. Feng, M. A. Katsoulakis, and D. G. Vlachos, Combining Uncertain Data and Expert Knowledge with Physics-Based Graphical Models for Quantifying Model Uncertainty (In Preparation)

N. R. Quiroz, J.L. Lansford, and D. G. Vlachos, Coupling Experimental Kinetics and Thermodynamic Modeling with IR Spectroscopy and Machine Learning for Fundamental Studies and Fast Product Quantification (In Preparation)

J. Feng, J. L. Lansford, M. A. Katsoulakis, and D. G. Vlachos, Probabilistic graph theory models combining physical models, expert opinion, and data. Proc. Nat. Acad. (In Preparation)

Invited Talks, Presentations and Posters

AIChE Meeting Presentation	**Orlando, FL**
Computational Modeling of operando Infrared Spectroscopy for Site-Specific Catalyst Characterization	Nov. 2019

- First place in the Catalysis and Reaction Engineering (CRE) Division poster competition for "Combining Experimental Kinetics, IR Spectroscopy and Machine Learning for Fast Product Quantification"

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 Surrogate 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	**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

- Won second place in the Fuels, Petrochemicals, and Energy Division

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 – saves 25-50 business hours per day
- Leveraged analysis and software development skills to automate identification of 17 high risk transactions
- Responded to audit of Capital One IRA team by generating dynamic alerts to all 900 branches

University Service & Leadership, Professional Affiliations

University of Virginia	**Charlottesville, VA**
University Dormitory Resident Advisor	2010 – 2013
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 piloted new experiments in Charlottesville elementary schools to teach science to low-income students

American Institute of Chemical Engineering (AICHE) Member	2010 – Present