

# Jacob R. Boes

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## Education

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### Carnegie Mellon University

PH.D. IN CHEMICAL ENGINEERING

Thesis: Multiscale Modeling of Adsorbate Interactions on Transition Metal Alloy Surfaces

Pittsburgh, PA

May 2017

### Michigan Technological University

B.S. IN CHEMICAL ENGINEERING, SUMMA CUM LAUDE

Minor in Hydrogen Fuel Cell Technologies

Houghton, MI

May 2012

## Research Experience

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### Stanford University, Chemical Engineering

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POST-DOCTORAL RESEARCHER

- Designing grey-box models for accurate prediction of co-adsorption across transition metals
- Implementing machine learning techniques for improved efficiency and reproducibility of computational catalysis techniques

Stanford, CA

2017 - present

### Carnegie Mellon University, Chemical Engineering

Adviser: John Kitchin

GRADUATE RESEARCHER

- Applied machine learning tools to the creation of atomistic potentials in high-dimensional alloy systems and developed methods for automating the process
- Compared the accuracy of existing atomistic potentials to those generated from machine learning tools for molecular dynamic and Monte-Carlo techniques
- Developed a thermodynamic model for predicting adsorption of small adsorbates on a segregating alloy surface
- Assisted in the development of tools and methodologies for more efficient means of sharing reproducible research

Pittsburgh, PA

2012 - 2017

### Michigan Technological University

Alternative Fuels Group

PRESIDENT AND CHAIR OF SOLAR COMMITTEE

- Established automated computational tools for the analysis of solar energy collection trends for the Keweenaw Research Center using Visual Basic
- Managed a team of four to investigate mechanical means of improving solar panel efficiency in snowy climates
- Constructed model in-floor heating system for testing as an energy efficient application of hydrogen fuel-cell byproducts with Dr. Jason Keith

Houghton, MI

2009 - 2010, 2011 - 2012

## Michigan Technological University, Chemical Engineering

### Adviser: David Shonnard

Houghton, MI

#### UNDERGRADUATE RESEARCHER

2011 - 2012

- Operated mass spectrometer for analysis of various pyrolyzed biostocks
- Researched and assisted in screening results by oil composition, accessibility, and environmental impact

### Adviser: Julia King

#### UNDERGRADUATE RESEARCHER

2008 - 2009

- Performed thermal, conductive, and mechanical experiments on various carbon nano-configuration containing resins
- Operated injection molder to produce various resin structures

## Publications (8 total)

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### First Author (5)

5. **Boes, J.R.** & Kitchin, J.R. (2017) "Modeling Segregation on AuPd(111) Surfaces with Density Functional Theory and Monte Carlo Simulations", *J. Phys. Chem. C.*, 121(6), 3479, doi:10.1021/acs.jpcc.6b12752.
4. **Boes, J.R.** & Kitchin, J.R. (2017) "Neural Network Predictions of Oxygen Interactions on a Dynamic Pd Surface", *Molecular Simulation*, 43, 346, doi:10.1080/08927022.2016.1274984.
3. **Boes, J.R.**, Groenenboom, M.C., Keith, J.A., & Kitchin, J.R. (2016) "Neural network and ReaxFF comparison for Au properties", *Int. J. Quantum Chem.*, 116(13), 979, doi:10.1002/qua.25115.
2. **Boes, J.R.**, Kondratyuk, P., Yin, C., Miller, J.B., Gellman, A.J., & Kitchin, J.R. (2015) "Core Level Shifts in Cu-Pd Alloys as a Function of Bulk Composition and Structure", *Surface Science*, 640, 127, doi:10.1016/j.susc.2015.02.011.
1. **Boes, J.R.**, Gumuslu, G., Miller, J.B., Gellman, A.J., & Kitchin, J.R. (2015) "Estimating Bulk-Composition-Dependent H<sub>2</sub> Adsorption Energies on Cu<sub>x</sub>Pd<sub>1-x</sub> Alloy (111) Surfaces", *ACS Catalysis*, 5(2), 1020, doi:10.1021/cs501585k.

### Co-Author (3)

3. Geng, F., **Boes, J.R.**, & Kitchin, J.R. (2017) "First-Principles Study of the Cu-Pd Phase Diagram", *Calphad*, 56, 224, doi:10.1016/j.calphad.2017.01.009.
2. Michael, J., Demeter, E.L., Illes, S.M., Fan, Q., **Boes, J.R.**, & Kitchin, J.R. (2015) "Alkaline Electrolyte and Fe Impurity Effects on the Performance and Active-phase Structure of NiOOH Thin Films for OER Catalysis Applications", *J. Phys. Chem. C*, 119(21), 11475, doi:10.1021/acs.jpcc.5b02458.
1. Gumuslu, G., Kondratyuk, P., **Boes, J.R.**, Morreale, B.D., Miller, J.M., Kitchin, J.R., & Gellman, A.J. (2015) "Correlation of Electronic Structure with Catalytic Activity: H<sub>2</sub>-D<sub>2</sub> Exchange across Cu<sub>x</sub>Pd<sub>1-x</sub> Composition Space", *ACS Catalysis*, 5(5), 3137, doi:10.1021/cs501586t.

## Selected Presentations

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### Contributed Talks

2017	<i>Neural Network Predictions of Segregation on AuPd(111) Surfaces,</i> Gordon Research Conference: Chemical Reactions at Surfaces	Barga LU, Italy
2016	<i>Neural Network and ReaxFF Comparison for Au Properties,</i> AIChE Annual Meeting	San Francisco, CA
2015	<i>Core Level Shifts in Cu-Pd Alloys as a Function of Bulk Composition and Structure,</i> AIChE Annual Meeting	Salt Lake City, UT
2014	<i>Estimating Bulk Composition Dependent H<sub>2</sub> Dissociative Adsorption Energies on Cu<sub>x</sub>Pd<sub>1-x</sub> Alloy (111) Surfaces,</i> AIChE Annual Meeting	Atlanta, GA

### Contributed Posters

2016	<i>Neural Network Predictions of Oxygen Interactions on a Dynamic Pd Surface,</i> AIChE Annual Meeting	San Francisco, CA
2016	<i>Practical Data Sharing for Molecular Simulation,</i> AIChE Annual Meeting	San Francisco, CA
2014	<i>Production of Purified Hydrogen as an Alternative Energy Source,</i> Andrew Carnegie Society	Pittsburgh, PA

### Honors & Awards

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2017	North American Catalysis Society Kokes Award	Denver, CO
2017	Ken Meyer Award for Excellence in Graduate Research in Chemical Engineering	CMU, PA
2015	ACS Summer Institute Certificate of Innovation	Washington, DC
2015	Mark Dennis Karl Outstanding Graduate Teaching Assistant Award	CMU, PA
2015	Bertucci Graduate Fellowship	CMU, PA
2014	Graduate Student Assembly Outstanding Representative Award	CMU, PA
2007-12	Presidential Scholarship	MTU, MI

### Selected Teaching Experience

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#### Carnegie Mellon University Kitchin Research Group

Pittsburgh, PA

#### MENTOR

2015 - 2016

- Assisted with mentoring of six masters students through published tutorials and frequent meetings contributing to the submission of three publications
- Instructed two undergraduate research students in basic molecular simulation techniques during weekly meetings

#### Chemical Engineering Department

#### TEACHING ASSISTANT

2012 - 2016

- Developed material based on student feedback for several lectures in graduate-level courses: Molecular Simulation and Chemical Reaction Engineering
- Designed and implemented three interactive recitations for MATLAB and held regular office hours as the mathematical software TA
- Completed grading and assisted during recitations for undergraduate-level courses: Introduction to Chemical Engineering and Thermodynamics

## **Michigan Technological University Chemistry Learning Center**

*Houghton, MI*

### **LEARNING CENTER COACH**

*2008 - 2012*

- Tutored individual students for 30-60 minute sessions once a week in physical, organic, and general chemistry
- Performed weekly reviews of general chemistry material for small teams, with a focus on self-education techniques
- Mentored other coaches on skills such as building off of existing understanding

## **Industry Experience**

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### **Domtar Paper Corporation**

*Rothschild, WI*

#### **PAPER MILL TECHNICAL INTERN**

*2010 - 2011*

- Performed regular product testing and ensured product specifications were being achieved
- Designed and implemented Visual Basic code for efficient data entry, storage, and retrieval in Excel
- Managed hourly workers on several plant projects

## **Selected Service and Outreach**

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### **Pittsburgh-Cleveland Catalysis Society**

*Pittsburgh, PA*

#### **SECRETARY**

*2015 - 2016*

- Contacted participants, gathered abstracts, and assembled the program for the 2016 annual meeting
- Managed the technical details of the event, including making a room reservation and ordering necessary food and equipment for approximately 50 attendees
- Created a temporary website to host organizational material for the meeting using WordPress; 300+ views during the week of the conference

### **Carnegie Mellon University, Chemical Engineering Graduate Student Association**

*Pittsburgh, PA*

#### **SYMPOSIUM CHAIR**

*2014 - 2015*

- Worked with a team of two others to organize the annual ChEGSA symposium, a conference for senior graduates to present their research to industrial guests
- Raised a record breaking \$11,000 from industrial and alumni donors
- Generated Python and LaTeX code capable of sending hundreds of personalized invitations to previous attendees

#### **VICE PRESIDENT**

*2014*

- Produced a \$9,000 budget for all Chemical engineering activities that year
- Converted the organizations financial information to entirely electronic documentation
- Reviewed and refined the organizations bylaws to eliminate antiquated procedures

# Carnegie Mellon University Graduate Student Assembly

Pittsburgh, PA

## GRADUATE STUDENT ASSEMBLY REPRESENTATIVE

2013 - 2014

- Represented Chemical Engineering interests at monthly meetings
- Founded service committee emphasizing student volunteer work in the community
- Organized first bike-advocacy day on campus

## Programming

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Python · SQL · LaTeX · Shell Script · MATLAB · MathCAD · Visual Basic

## References

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### John Kitchin, Professor

Chemical Engineering  
Carnegie Mellon University

☎ (412) 268-7803, ✉ [jkitchin@andrew.cmu.edu](mailto:jkitchin@andrew.cmu.edu)

### James Miller, Senior Scientist

Chemical and Biological Engineering  
University of Wisconsin-Madison

☎ (608) 886-7819, ✉ [james.miller@wisc.edu](mailto:james.miller@wisc.edu)

### Andrew Gellman, Lord Professor

Chemical Engineering  
Carnegie Mellon University

☎ (412) 268-3848, ✉ [gellman@cmu.edu](mailto:gellman@cmu.edu)

### Zachary Ulissi, Assistant Professor

Chemical Engineering  
Carnegie Mellon University

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