Jacob R. Boes

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Education

Carnegie Mellon University
Pittsburgh, PA

PH.D. CANDIDATE IN CHEMICAL ENGINEERING
May 2017

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

Michigan Technological University
Houghton, MI

B.S. IN CHEMICAL ENGINEERING, SUMMA CUM LAUDE
May 2012

Minor in Hydrogen Fuel Cell Technologies

Research Experience

Stanford University, Chemical Engineering
SUNCAT
Stanford, CA

POST-DOCTORAL RESEARCHER
2017 - present

- 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

Carnegie Mellon University, Chemical Engineering
Adviser: John Kitchin
Pittsburgh, PA

GRADUATE RESEARCHER
2012 - 2017

- 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

Michigan Technological University
Alternative Fuels Group
Houghton, MI

PRESIDENT AND CHAIR OF SOLAR COMMITTEE
2009 - 1010, 2011 - 2012

- 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

Publications (8 total)

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_2 Adsorption Energies on Cu_xPd_{1-x} 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_2-D_2 Exchange across Cu_xPd_{1-x} Composition Space", *ACS Catalysis*, 5(5), 3137, doi:10.1021/cs501586t.

Selected Presentations

Contributed Talks

2017	*Neural Network Predictions of Segregation on AuPd(111) Surfaces*, Gordon Research Conference: Chemical Reactions at Surfaces	*Barga LU, Italy*
2016	*Neural Network and ReaxFF Comparison for Au Properties*, AIChE Annual Meeting	*San Francisco, CA*
2015	*Core Level Shifts in Cu-Pd Alloys as a Function of Bulk Composition and Structure*, AIChE Annual Meeting	*Salt Lake City, UT*
2014	*Estimating Bulk Composition Dependent H_2 Dissociative Adsorption Energies on Cu_xPd_{1-x} Alloy (111) Surfaces*, AIChE Annual Meeting	*Atlanta, GA*

Contributed Posters

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

Honors & Awards

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

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

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

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 alumi 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

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

References

John Kitchin, Professor
Chemical Engineering
Carnegie Mellon University
(412) 268-7803, jkitchin@andrew.cmu.edu

Andrew Gellman, Lord Professor
Chemical Engineering
Carnegie Mellon University
(412) 268-3848, gellman@cmu.edu

James Miller, Senior Scientist
Chemical and Biological Engineering
University of Wisconsin-Madison
(608) 886-7819, james.miller@wisc.edu

Zachary Ulissi, Assistant Professor
Chemical Engineering
Carnegie Mellon University
(301) 547-3450, zulissi@andrew.cmu.edu