

JOE GOMES

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([Google Scholar](#))

ACADEMIC APPOINTMENTS

- University of Iowa** *2019-Present*
Assistant Professor: Chemical and Biochemical Engineering
- Stanford University** *2015-2019*
Postdoctoral Fellow: Chemistry (2015-2018), Bioengineering (2018-2019)
Advisor: Prof. Vijay Pande

EDUCATION

- University of California Berkeley** *2008-2015*
PhD: Chemical Engineering
Advisors: Prof. Alexis T. Bell and Prof. Martin Head-Gordon
Thesis: *Theoretical Simulations of Zeolite-Catalyzed Reactions*
- University of Illinois Chicago** *2004-2008*
BSc.: Chemical Engineering
Advisor: Prof. Randall Meyer and Prof. John Regalbuto

PUBLICATIONS

18. Weihau Hu, Bowen Liu, **Joseph Gomes**, Marinka Zitnik, Percy Liang, Vijay S. Pande, Jure Leskovec. "Pre-training Graph Neural Networks" submitted. Preprint [arXiv](#), **2019**.
17. Rishi Sharma, Amir Barati Farimani, **Joseph Gomes**, Peter Eastman, Vijay S. Pande. "Weakly-Supervised Deep Learning of Heat Transport via Physics Informed Loss" submitted. Preprint [arXiv](#), **2018**.
16. **Joseph Gomes***, Amir Barati Farimani*, Rishi Sharma, Franklin L. Lee, Vijay S. Pande. "Deep Learning Phase Segregation" submitted. Preprint [arXiv](#), **2018**.(* denotes equal authorship)
15. **Joseph Gomes***, Amir Barati Farimani*, Vijay S. Pande. "Deep Learning the Physics of Transport Phenomena" submitted. Preprint [arXiv](#), **2017**. Featured in: [Nature Physics](#)
14. **Joseph Gomes***, Bharath Ramsundar*, Evan N. Feinberg, Vijay S. Pande. "Atomic Convolutional Networks for Predicting Protein-Ligand Binding Affinity" submitted. Preprint [arXiv](#), **2017**.
13. Zhenqin Wu, Bharath Ramsundar, Evan N. Feinberg, **Joseph Gomes**, Caleb Geniesse, Aneesh S. Pappu, Karl Leswing, Vijay S. Pande. "Moleculenet: A Benchmark for Molecular Machine Learning" **Chemical Science**, 9, 513-530, **2018**. Featured in: [ChemistryWorld](#)
12. Bowen Liu, Bharath Ramsundar, Prasad Kawthekar, Jade Shi, **Joseph Gomes**, Quang Luu Nguyen, Stephen Ho, Jack Sloane, Paul Wender, Vijay Pande. "Retrosynthetic Reaction Prediction using Neural Sequence-to-Sequence Models" **ACS Central Science**, 3, 1103-1113, **2018**.
11. Lee-Ping Wang, Keri A. McKiernan, **Joseph Gomes**, Kyle A. Beauchamp, Teresa Head-Gordon, Julia E. Rice, William C. Swope, Todd J. Martínez, Vijay S. Pande. "Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15", **Journal of Physical Chemistry B**, 121, 4023-4039, **2017**.

10. Diana C. Tranca, Paul M. Zimmerman, **Joseph Gomes**, Daniel S. Lambrecht, Frerich J. Keil, Martin Head-Gordon, Alexis T. Bell. "Hexane Cracking on ZSM-5 and Faujasite Zeolites: a QM/MM/QCT Study", **Journal of Physical Chemistry C**, 119, 28836-28853, **2015**.
9. Shylesh Sankaranarayananpillai, Sanil Sreekumar, **Joseph Gomes**, Adam Grippo, George E. Arab, Martin Head-Gordon, F. Dean Toste, Alexis T. Bell. "Catalytic Upgrading of Biomass-Derived Methyl Ketones to Transportation Fuel Precursors by an Organocatalytic Approach", **Angewandte Chemie International Edition**, 54, 4673-4677, **2015**.
8. Sankaranarayananpillai Shylesh, David Hanna, **Joseph Gomes**, Christian G. Canlas, Martin Head-Gordon, Alexis T. Bell. "The Role of Hydroxyl Group Acidity on the Activity of Silica-Supported Secondary Amines for the Self-Condensation of *n*-Butanal", **ChemSusChem**, 8, 466-472, **2015**. (Back Cover)
7. Yi-Pei Li, **Joseph Gomes**, Shaama Mallikarjun Sharada, Alexis T. Bell, Martin Head-Gordon. "Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies", **Journal of Physical Chemistry C**, 119, 1840-1850, **2015**.
6. Yihan Shao, et. Al. "Advances in Molecular Quantum Chemistry Contained in the Q-Chem 4 Program Packages", **Molecular Physics**, 113, 184-215, **2015**.
5. **Joseph Gomes**, Martin Head-Gordon, Alexis T. Bell. "Reaction Dynamics of Alkene Methylation by Methanol over H-MFP", **Journal of Physical Chemistry C**, 37, 21409-21419, **2014**.
4. Sankaranarayananpillai Shylesh, David Hanna, **Joseph Gomes**, Siddarth Krishna, Christian G. Canlas, Martin Head-Gordon, Alexis T. Bell. "Tailoring the Co-operative Acid-Base Effects in Silica Supported Amine Catalysts: Applications in the Continuous Gas-Phase Self Condensation of *n*-Butanal", **ChemCatChem**, 6, 1283-1290, **2014**.
3. Andreas W. Hauser, **Joseph Gomes**, Michal Bajdich, Martin Head-Gordon, Alexis T. Bell. "Subnanometer-Sized Pt/Sn Alloy Cluster Catalysts for the Dehydrogenation of Linear Alkanes", **Physical Chemistry Chemical Physics**, 15, 20727-20734, **2013**.
2. Paul M. Zimmerman, Diana C. Tranca, Joseph Gomes, Daniel S. Lambrecht, Martin Head-Gordon, Alexis T. Bell. "Ab Initio Simulations Reveal that Reaction Dynamics Strongly Affect Product Selectivity for the Cracking of Alkanes over H-MFP", **Journal of the American Chemical Society**, 134, 19468-19476, **2012**.
1. **Joseph Gomes**, Paul M. Zimmerman, Martin Head-Gordon, Alexis T. Bell. "Accurate Prediction of Hydrocarbon Interactions with Zeolites Utilizing Improved Exchange-Correlation Functionals and QM/MM Methods", **Journal of Physical Chemistry C**, 116, 15406-15414, **2012**.

INVITED TALKS

Joseph Gomes. "Deep Learning in the Physical Sciences". Presented at Department of Chemical Engineering, University of Washington, Seattle, WA, United States, March 4, 2019.

Joseph Gomes. "Deep Learning in the Physical Sciences". Presented at Department of Chemical and Biochemical Engineering, University of Iowa, Iowa City, IA, United States, February 12, 2019.

Joseph Gomes. "Deep Learning Physical Phenomena". Presented at Data & Analytics Services Group, National Energy Research Scientific Computing Center, Lawrence Berkeley National Lab, Berkeley, CA, United States, July 6, 2018.

CONFERENCE PRESENTATIONS

Joseph Gomes. "**Data-Driven Modeling in Molecular Science and Chemical Engineering**". Presented at the 2018 AIChE Annual Meeting, Pittsburgh, PA, United States, October 28-November 2, 2018.

Joseph Gomes, Vijay S. Pande. "**Deep Learning Physical Phenomena**". Presented at the 2018 AIChE Annual Meeting, Pittsburgh, PA, United States, October 28-November 2, 2018.

Zhenqin Wu, Bharath Ramsundar, Evan N. Feinberg, Joseph Gomes, Caleb Geniesse, Aneesh S. Pappu, Karl Leswing, Vijay S. Pande. "**Moleculenet: A Benchmark for Molecular Machine Learning**". Presented at the 2018 AIChE Annual Meeting, Pittsburgh, PA, United States, October 28-November 2, 2018.

Joseph Gomes, Vijay S. Pande. "**Building Better Water Force Fields: A Systematic and Reproducible Optimization of 3- and 4-Point Water Models with an Improved Nonbonded Functional Form**". Presented at the 2018 AIChE Annual Meeting, Pittsburgh, PA, United States, October 28-November 2, 2018.

Joseph Gomes, Amir Barati Faramani, Vijay S. Pande. "**Deep Learning Physical Phenomena**". Presented at the 2018 APS March Meeting, Los Angeles, CA, United States, March 5-9, 2018.

Joseph Gomes, Martin Head-Gordon, Alexis T. Bell. "**Theoretical Studies of Propene Oligomerization in Ni-Na-X**". Presented at the 2013 AIChE Annual Meeting, San Francisco, CA, United States, November 3-8, 2013.

Joseph Gomes, Martin Head-Gordon, Alexis T. Bell. "**Application of DFT-D and QM/MM Methods in Zeolite-Catalyzed Reactions**". Presented at the 2013 AIChE Annual Meeting, San Francisco, CA, United States, November 3-8, 2013.

Joseph Gomes, Martin Head-Gordon, Alexis T. Bell. "**Reaction Dynamics of Alkene Methylation in H-MFI**". Presented at the 23rd North American Meeting of the Catalysis Society, Louisville, KY, United States, June 2-7, 2013.

Joseph Gomes, Martin Head-Gordon, Alexis T. Bell. "**Application of Improved Exchange-Correlation Functionals: Chemical Accuracy in Computational Catalysis**". Presented at the 22nd North American Meeting of the Catalysis Society, Detroit, MI, United States, June 5-10, 2011.

Joseph Gomes, Martin Head-Gordon, Alexis T. Bell. "**Theoretical Studies of Alkene Isomerization and Dimerization in Zeolites**". Presented at the 2010 AIChE Annual Meeting, Salt Lake City, UT, United States, November 7-12, 2010.

AWARDS

Heinz Heinemann Prize for Graduate Research in Catalysis	2012
Outstanding Graduate Student Instructor	2012
AIChE McCormack Award	2008
Leonard Kotin Memorial Award for Excellence in Physical Chemistry	2007
Olive C. and Alfred L. Koehn Scholarship	2007

TEACHING EXPERIENCE

- Teaching Assistant, **Transport Phenomena**, University of California Berkeley, 2011.
- Teaching Assistant, **Mathematical Methods in Chemical Engineering**, University of California Berkeley, 2009.

ACADEMIC SERVICES

- **Reviewer** for the following journals:

ACS Catalysis, Molecular Physics, Journal of Physical Chemistry C

- **Chair:** Accelerated Materials Discovery, Machine Learning for Energy Materials Discovery, Harvard University, May 2017.
- **Chair:** Computational Catalysis II, Annual Meeting of the AIChE, San Francisco, November 2014.

PROFESSIONAL SOCIETIES MEMBERSHIP

- American Institute of Chemical Engineering (AIChE) *2007-Present*
- American Chemical Society (ACS) *2012-Present*
- American Physical Society (APS) *2017-Date*