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 Sankaranarayanapillai, 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. Sankaranarayanapillai 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-MFI*", **Journal of Physical Chemistry C**, 37, 21409-21419, **2014**.

4. Sankaranarayanapillai 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-MFI*", **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*