# Matthew D. Witman, Ph.D.

Computational Material Scientist · Data Scientist · Chemical Engineer

*Sandia National Laboratories, 7011 East Ave, Livermore, CA 94550*

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## Summary

Applies a diverse computational skill set to solve problems and make new discoveries at the intersection of material science, statistics, computer science, and machine learning. Thrives working in a team environment, proactively leads international collaborations to complete challenging research objectives, and effectively communicates technical concepts.

## Education

**University of California, Berkeley** *Berkeley, CA*

Ph.D. Chemical Engineering *08/2014 - 05/2019*

- Advisor: Prof. Berend Smit

**École Polytechnique Fédérale de Lausanne** *Sion, Switzerland*

Visiting Ph.D. Researcher *06/2015 - 05/2019*

- Advisor: Prof. Berend Smit

**Schreyer Honors College, The Pennsylvania State University** *State College, PA*

B.Sc. Chemical Engineering (*Summa Cum Laude*) *08/2009 - 12/2013*

- Honors thesis research advisor: Prof. Enrique Gomez

## Experience

**Sandia National Laboratories** *Livermore, CA*

Postdoctoral Researcher (Mentors: Mark Allendorf and Anthony McDaniel) *June 2019 - Current*

- Main Project: "Discovery of high-performance hydrogen storage and generation materials via data-driven approaches"
- Developed machine/deep learning techniques and computational workflows to (1) tractably predict, simulate, or high-throughput screen materials for hydrogen storage and generation and (2) direct the efficient selection and experimental validation of high potential candidates.

**Sunchem, LLC** *Concord, CA*

Technical Consultant *April 2020 - Current*

- Modeled and numerically solved the coupled partial differential equations for combined diffusion and reaction of gold ions in MOF/polymer composites at the continuum scale.
- Significantly reduced the startup's costs by utilizing only open source code, rather than commercial solvers, to provide process optimization insights and profitability projections.

**UC Berkeley - Dept of Chemical Engineering** *Berkeley, CA*

Graduate Student Researcher (Adviser: Prof. Berend Smit) *08/2014 - 05/2019*

- Dissertation: "Computationally advancing the predictive power of the nanoporous materials genome"
- Developed and applied computational approaches (statistical mechanics, graph theory, and data science techniques) to more efficiently simulate and discover high-performance nanoporous materials for energy related applications.

**Pennsylvania State University - Dept of Chemical Engineering** *State College, PA*

Undergraduate Researcher Assistant (Adviser: Prof. Enrique Gomez) *06/2011 - 12/2013*

- Honors Thesis: "Conjugated block copolymers in organic photovoltaics
- Elucidated how lamellar, microphase separated active layers in organic solar cells could optimize device performance and produce record performance in all-polymer active layers.

**General Electric, Inc.** *Twinsburg, OH*

Process Engineering Intern *06/2013 - 08/2013*

- Coded VBA applications to automate processing and dissemination of the supply chain data from an underutilized $20 MM Enterprise Resource Planning investment.

**Janssen Pharmaceutical of Johnson & Johnson** *Raritan, NJ*

Supply Chain Management Co-op *06/2012 - 12/2012*

- Coded VBA programs that (1) automated supply chain workflows and reduced man hour requirements by 80% for US demand planners, (2) identified poor alignments between financial and operating forecasts of Janssen's multi-billion dollar Tier 1 product portfolio, and (3) automated statistical forecasting of established products' demand to improve inventory levels.

## Publications

### Published

M. Witman, G. Ek, S. Ling, J. Chames, S. Agarwal, J. Wong, M. D. Allendorf, M. Sahlberg, and V. Stavila, *Data-Driven Discovery and Synthesis of High Entropy Alloy Hydrides with Targeted Thermodynamic Stability*, Chem. Mater., (2021), p. acs.chemmater.1c00647

M. D. Allendorf, V. Stavila, M. Witman, C. K. Brozek, and C. H. Hendon, *What Lies beneath a Metal–Organic Framework Crystal Structure? New Design Principles from Unexpected Behaviors*, J. Am. Chem. Soc., (2021), p. jacs.0c10777

A. Datar, M. Witman, and L.-C. Lin, *Improving Computational Assessment of Porous Materials for Water Adsorption Applications via Flat Histogram Methods*, J. Phys. Chem. C, (2021), p. acs.jpcc.0c11082

M. Witman, S. Ling, D. M. Grant, G. S. Walker, S. Agarwal, V. Stavila, and M. D. Allendorf, *Extracting an Empirical Intermetallic Hydride Design Principle from Limited Data via Interpretable Machine Learning*, J. Phys. Chem. Lett., 11 (2020), pp. 40–47

M. Witman, S. Ling, V. Stavila, P. Wijeratne, H. Furukawa, and M. D. Allendorf, *Design principles for the ultimate gas deliverable capacity material: nonporous to porous deformations without volume change*, Mol. Syst. Des. Eng., 5 (2020), pp. 1491–1503

N. A. Mahynski, H. W. Hatch, M. Witman, D. A. Sheen, J. R. Errington, and V. K. Shen, *Flat-histogram extrapolation as a useful tool in the age of big data*, Mol. Simul., 7022 (2020), pp. 1–13

G. Ek, M. M. Nygård, A. F. Pavan, J. Montero, P. F. Henry, M. H. Sørby, M. Witman, V. Stavila, C. Zlotea, B. C. Hauback, and M. Sahlberg, *Elucidating the Effects of the Composition on Hydrogen Sorption in TiVZrNbHf-Based High-Entropy Alloys*, Inorg. Chem., 60 (2021), pp. 1124–1132

M. Witman, D. Gidon, D. B. Graves, B. Smit, and A. Mesbah, *Sim-to-real transfer reinforcement learning for control of thermal effects of an atmospheric pressure plasma jet*, Plasma Sources Sci. Technol., 28 (2019), p. 095019

S. Jawahery, N. Rampal, S. M. Moosavi, M. Witman, and B. Smit, *Ab Initio Flexible Force Field for Metal–Organic Frameworks Using Dummy Model Coordination Bonds*, J. Chem. Theory Comput., 15 (2019), pp. 3666–3677

M. Witman, S. Ling, P. Boyd, S. Barthel, M. Haranczyk, B. Slater, and B. Smit, *Cutting Materials in Half: A Graph Theory Approach for Generating Crystal Surfaces and Its Prediction of 2D Zeolites*, ACS Cent. Sci., 4 (2018), pp. 235–245

M. Witman, N. A. Mahynski, and B. Smit, *Flat-Histogram Monte Carlo as an Efficient Tool To Evaluate Adsorption Processes Involving Rigid and Deformable Molecules*, J. Chem. Theory Comput., 14 (2018), pp. 6149–6158

M. Witman, S. Ling, A. Gladysiak, K. C. Stylianou, B. Smit, B. Slater, and M. Haranczyk, *Rational Design of a Low-Cost, High-Performance Metal–Organic Framework for Hydrogen Storage and Carbon Capture*, J. Phys. Chem. C, 121 (2017), pp. 1171–1181

M. Witman, S. Ling, S. Jawahery, P. G. Boyd, M. Haranczyk, B. Slater, and B. Smit, *The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials*, J. Am. Chem. Soc., 139 (2017), pp. 5547–5557

S. Jawahery, C. M. Simon, E. Braun, M. Witman, D. Tiana, B. Vlaisavljevich, and B. Smit, *Adsorbate-induced lattice deformation in IRMOF-74 series*, Nat. Commun., 8 (2017), p. 13945

P. G. Boyd, S. M. Moosavi, M. Witman, and B. Smit, *Force-Field Prediction of Materials Properties in Metal-Organic Frameworks*, J. Phys. Chem. Lett., 8 (2017), pp. 357–363

D. Ongari, P. G. Boyd, S. Barthel, M. Witman, M. Haranczyk, and B. Smit, *Accurate Characterization of the Pore Volume in Microporous Crystalline Materials*, Langmuir, 33 (2017), pp. 14529–14538

M. Witman, S. Ling, S. Anderson, L. Tong, K. C. Stylianou, B. Slater, B. Smit, and M. Haranczyk, *In silico design and screening of hypothetical MOF-74 analogs and their experimental synthesis*, Chem. Sci., 7 (2016), pp. 6263–6272

C. Guo, Y.-H. Lin, M. Witman, K. A. Smith, C. Wang, A. Hexemer, J. Strzalka, E. D. Gomez, and R. Verduzco, *Conjugated Block Copolymer Photovoltaics with near 3% Efficiency through Microphase Separation*, Nano Lett., 13 (2013), pp. 2957–2963

### Under Review

C. Spataru, M. Witman, and R. Jones, *Tuning the critical Li intercalation concentrations for MoX2 bilayer phase transitions using classical and machine learning approaches*, Submitted, (2021)

M. Allendorf, J. L. Snider, V. Stavila, M. Witman, and Bowden, *Chemical Goldilocks Challenges for Transport and Storage of Hydrogen*, Submitted, (2021)

## Awards, Fellowships, & Grants

2020 **MSD&E HOT Article**, Molecular Systems Design & Engineering

2020 **Sci-Mix Selection**, ACS Division of Chemical Information

2020 **Spot Award**, Sandia National Laboratories

2017 **Thomas Young Centre Junior Research Fellowship**, University College London

2016 **Peder Sather Fellowship**, UC Berkeley

2013 **Lee and Mary Eagleton Award for Excellence in Design**, Pennsylvania State University

2012 **Platinum Encore Award**, Johnson and Johnson
**Bronze Encore Award**, Johnson and Johnson

2011 **NSF-REU Fellowship**, Pennsylvania State University

## Presentations

### Invited Talks

Witman, M et al. 2021. *A data driven road map for the discovery of optimal hydrogen storage alloys.* Invited talk: MRS Fall Meeting, Boston, MA.

Witman, M et al. 2021. *Accelerating data-driven discovery of materials for hydrogen storage and generation.* Invited talk: HFTO Postdoctoral Award Symposium, Virtual.

Witman, M et al. 2020. *Discovering new hydrogen storage materials using an empirical design principle for metal hydrides*. Invited lightning talk: MRS Spring/Fall Meeting, Virtual

Witman, M et al. 2019. *Graph theoretic construction of crystal surfaces and its prediction of 2D zeolites*. Invited poster: EFRC PI Meeting, Washington, D.C.

Witman, M et al. 2017. *The influence of intrinsic framework flexibility on adsorption in nanoporous materials.* Invited poster: EFRC PI Meeting, Washington, D.C.

### Contributed Presentations

Witman, M et al. 2021. Data-driven discovery of high entropy alloy hydrides with targeted thermodynamic stability. Oral presentation: New Mexico Machine Learning Symposium, Virtual.

Witman, M et al. 2021. Data-driven discovery of high entropy alloy hydrides with targeted thermodynamic stability. Oral presentation: 14$^{th}$ Annual Sandia Postdoctoral Technical Showcase, Virtual.

Witman, M et al. 2020. Extracting an empirical intermetallic hydride design principle from limited data via interpretable machine learning. Oral presentation: ACS Spring Meeting.

Witman, M et al. 2020. Identification of previously untested, high-potential $H_2$ physisorbents via graph theory-based descriptors of MOF flexibility. Oral presentation: ACS Spring Meeting.

Witman, M. 2019. Computationally advancing the predictive power of the nanoporous materials genome. Departmental seminar: UC Berkeley, CA.

Witman, M et al. 2018. Cutting materials in half: a graph theory approach to generating crystal surfaces and its prediction of 2D zeolites. Oral presentation: AIChE National Meeting, Pittsburgh, PA.

Witman, M et al. 2017. The influence of intrinsic framework flexibility on adsorption in nanoporous materials. Oral presentation: AIChE National Meeting, Minneapolis, MN.

Witman, M et al. 2016. *In silico* design and screening of hypothetical MOF-74 analogs and their experimental synthesis. Oral presentation: AIChE National Meeting, San Francisco, CA.

## Teaching Experience

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| Fall 2017 | **Chemical Kinetics and Reaction Engineering**, Graduate Student Instructor | *UC Berkeley* |
| Fall 2015 | **Chemical Kinetics and Reaction Engineering**, Graduate Student Instructor | *UC Berkeley* |
| Fall 2014 | **Chemical Engineering Laboratory**, Graduate Student Instructor | *UC Berkeley* |

## Mentoring

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| 2020- | **Grace Lu**, Graduate Student Researcher, University of Illinois at Urbana-Champaign |
| 2020- | **Archit Datar**, Graduate Student Researcher, Ohio State University |
| 2018-2019 | **Bradley Wright**, Undergraduate Researcher, UC Berkeley |

## Outreach & Professional Development

### Service and Outreach

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| 2021- | **I-Art-Science**, Creator | *Virtual* |
| 2020- | **Protect Our Winters**, Volunteer | *Virtual* |
| 2017-2019 | **Bay Area Scientists in Schools**, Volunteer Educator | *Berkeley* |

### Peer Review

Joule, Angewandte Chemie International Edition, Chemistry of Materials, Journal of Materials Chemistry A, Journal of Chemical Physics, and Patterns