Mathew D. Witman, Ph.D.

Computational Material Scientist · Data Scientist · Chemical Engineer

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Summary

I am interested in applying my data science skills to solve problems and make new discoveries at the intersection of statistics, computer science, and machine learning. These are skills that I have developed and applied to computational materials science research throughout my PhD and previous work experiences. I thrive working in a team environment and have proactively collaborated with researchers at many different institutions around the world to complete challenging projects.

Education

University of California, Berkeley — *Berkeley, CA*

Ph.D. Candidate in the Department of Chemical & Biomolecular Engineering (GPA: 3.92) — *Sep. 2014 - May 2019*

École Polytechnique Fédérale de Lausanne — *Switzerland*

Visiting Ph.D. Researcher — *Jun. 2015 - May 2019*

Schreyer Honors College at the Pennsylvania State University — *State College, PA*

B.Sc. in Chemical Engineering (*Summa Cum Laude*, GPA: 3.95) — *Sep. 2009 - Dec. 2013*

Chemical engineering semester study abroad (*University of Bath, UK*) — *Spring 2011*

Technical Skills & Software

Programming	EXPERT: Python, NumPy, SciPy, Bash
	PROFICIENT: Tensorflow/Keras, C/C++, HTML/CSS, Matlab/Mathematica, SQL, VBA, Blender, LaTex, Aspen HYSYS
nearmincut	Author: Implementing a recursive solution to the all-near-min-cut problem
ColorBooked	Author: Image processing and unsupervised learning for automated coloring book image generation
LammpsInterface	Co-author: Interpreting crystalline materials as graphs for high-throughput interfacing to molecular dynamics codes
AMP	Contributor: Deep neural network modeling of *ab initio* potential energy surfaces

Experience

Laboratory of Molecular Simulation (UC Berkeley, Berend Smit Group) — *Berkeley, CA*

Graduate Student Researcher, Instructor, and Mentor — *Jan. 2015 - May 2019*

- **Applied reinforcement learning techniques** to transition state sampling in chemical systems.
- **Trained deep neural network models** of atomic interactions in zeolites to significantly reduce the computational expense of molecular dynamics simulations while retaining quantum chemical accuracy.
- **Coded a recursive, minimal cut graph theory algorithm** to perform high-throughput data analysis and identify materials with previously unrecognized potential for 2-dimensional synthesis and application in water desalination.
- **Derived and programmed enhanced Monte Carlo sampling schemes** to efficiently generate more and better statistical information when performing high-throughput materials screening for adsorption applications involving flexible chain molecules.
- **Utilized cheminformatics and computer vision techniques** to perform hypothetical crystal structure prediction in the search for novel, high-performing adsorbents.
- **Developed statistical physics models and high-throughput screening techniques** to identify systematic biases that arise when simulating adsorption in flexible materials.

General Electric, Inc. — *Twinsburg, OH*

Process Engineering Intern — *Jun. 2013 - Aug. 2013*

- **Coded VBA applications** to automate the Returned Materials Authorization process and capitalize on an underutilized $20 MM Enterprise Resource Planning investment.

Janssen (A Pharmaceutical Company of Johnson & Johnson) *Raritan, NJ*

Customer Management Co-op *Jun. 2012 - Dec. 2012*

- **Wrote VBA programs to optimize data acquisition and demand planning analysis** for the US Sales & Operations supply chain team to improve reporting accuracy and reduce monthly man hour requirements by 80% in a constrained work stream.
- **Managed the monthly Executive Sales & Operations Planning Dashboard:** automated the identification of poor alignments between financial and operating forecasts of Janssen's multi-billion dollar Tier 1 product portfolio to create actionable intelligence for the North America leadership team.
- **Implemented an automated statistical forecasting tool** to monitor over 200 established pharmaceutical products which yielded improved forecast/demand alignment and inventory levels.

PSU Department of Chemical Engineering (Enrique Gomez Group) *State College, PA*

Undergraduate Researcher *Jun. 2011 - Dec. 2013*

- **Constructed a block co-polymer organic photovoltaic device** with record 3% efficiency due to a microphase separated active layer.
- **Built, tested, and optimized** organic electronic devices such as photovoltaic cells and transistors for 2+ years.

Publications & Awards

Publications:

2018 M. Witman, N. A. Mahynski, and B. Smit, *Flat-histogram Monte Carlo simulations as an efficient tool to evaluate adsorption processes involving rigid and deformable molecules*, submitted, (2018)

2018 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

2017 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

2017 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

2017 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

2017 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

2017 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

2016 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

2013 C. Guo, Y.-H. Lin, M. D. 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

Awards:

2017 **Thomas Young Centre Junior Research Fellowship**, Outstanding research project with a UK institution *London, UK*

2016 **Peder Sather Fellowship**, Outstanding research project between UC Berkeley and a Norwegian institution *Berkeley, CA*

2013 **Eagleton Design Award**, Best chemical plant design project among 2013 class of PSU chemical engineers *State College, PA*

2012 **Platinum and Bronze Encore Awards**, Outstanding performance at Johnson & Johnson *Raritan, NJ*

2011 **NSF-REU Fellowship**, Award to study organic photovoltaics at PSU *State College, PA*

Interests

Coursera Classes Machine Learning, Design of Algorithms I & II, Interactive Programming in Python I & II, Data Science at Scale (*in progress*), Deeplearning.ai Specialization (*in progress*)

Berkeley Classes Reinforcement Learning, Statistical Mechanics I & II, Transport Phenomena, Reaction Engineering, Thermodynamics

Languages French (Niveau B1/B2)

Outreach Bay Area Scientists in Schools (BASIS)

Hobbies Mountaineering, Snowboarding, Backpacking, Soccer, Art, Travel, Saxophone, Piano

More About Me My personal web page and adventure blog: `https://mwitman1.github.io`