

## Education

2012

2016

**Ph.D. Chemical Engineering**, *University of California, Berkeley*.

Topic: screening large databases of nanoporous materials for storing and separating gases using statistical mechanical models, molecular simulations, and machine learning

Supervisor: Berend Smit

GPA: 3.7/4.0.

2010

2012

**Ph.D. Mathematics**, *University of British Columbia*.

Topic: understanding how a protein signaling network orchestrates cellular wound healing using mathematical models

Supervisor: Leah Keshet

Passed qualifying exams. Course average: 93.6%.

2005

2010

**B.S. Chemical Engineering**, *The University of Akron*.

*Summa Cum Laude*. GPA: 3.993/4.0

Minor: Applied mathematics

## Peer-reviewed publications

Google Scholar Profile

20. **C. Simon**, E. Braun, C. Carraro, B. Smit. Statistical mechanical model of gas adsorption in porous crystals with dynamic moieties. *Proc. Natl. Acad. Sci.* (2017) DOI
19. S. Elsaïdi, M. Mohamed, **C. Simon**, E. Braun, T. Pham, K. Forrest, W. Xu, D. Banerjee, B. Space, M. Zaworotko, P. Thallapally. Effects of Ring Rotation upon Gas Adsorption in Pillared Square Grid Networks. *Chem. Sci.* (2017) DOI
18. S. Jawahery, **C. Simon**, E. Braun, M. Witman, D. Tiana, B. Vlaisavljevich, B. Smit. Adsorbate-induced lattice deformation in the IRMOF-74 series. *Nat. Comm.* (2017) DOI
17. A. Thornton, **C. Simon**, J. Kim, O. Kwon, K. Deeg, K. Konstas, S. Pas, M. Hill, D. Winkler, M. Haranczyk, B. Smit. The Materials Genome in action: identifying the performance limits of physical hydrogen storage. *Chem. Mater.* (2017) DOI
16. R. Patil, D. Banerjee, **C. Simon**, J. Atwood, P. Thallapally. Noria, a highly Xe-selective Nanoporous Organic Solid. *Chem. Eur. J.* (2016) DOI Press coverage: Frontispiece, Hot paper, Chemistry Views
15. D. Banerjee, **C. Simon**, A. Plonka, R. Motkuri, J. Liu, X. Chen, B. Smit, J. Parise, M. Haranczyk, P. Thallapally. Metal-Organic Framework with Optimal Adsorption, Separation, and Selectivity towards Xenon. *Nat. Comm.* (2016) DOI  
Press coverage: LBL, EPFL, Research Gate, Chemical & Engineering News
14. D. Gomez-Gualdrón, **C. Simon**, W. Lassman, D. Chen, R. L. Martin, M. Haranczyk, O. K. Farha, B. Smit, R. Q. Snurr. Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials. *Chem. Eng. Sci.* (2016) DOI
13. **C. Simon**, B. Smit, M. Haranczyk. pyIAST: Ideal Adsorbed Solution Theory (IAST) Python package. *Comput. Phys. Commun.* (2016) DOI
12. **C. Simon**, R. Mercado, S. K. Schnell, B. Smit, and M. Haranczyk. What Are the Best Materials To Separate a Xenon/Krypton Mixture? *Chem. Mater.* (2015) DOI
11. **C. Simon**, J. Kim, D. Gomez-Gualdrón, J. Camp, Y. Chung, R. L. Martin, R. Mercado, M.W. Deem, D. Gunter, M. Haranczyk, D. Sholl, R. Snurr, B. Smit. The Materials Genome in Action: Identifying the Performance Limits to Methane Storage. *Energy Environ. Sci.* (2015) DOI Inside front cover art.  
Press coverage: Chemistry World, EPFL
10. Y. Bao, R. L. Martin, **C. Simon**, M. Haranczyk, B. Smit, and M.W. Deem. In Silico Discovery of High Deliverable Capacity Metal-Organic Frameworks. *J. Phys. Chem. C*. (2014) DOI
9. D. Feng, K. Wang, Z. Wei, Y.P. Chen, **C. Simon**, R. Arvapally, R.L. Martin, M. Bosch, T.F. Liu, S. Fordham, D. Yuan, M.A. Omary, M. Haranczyk, B. Smit, H.C. Zhou. Kinetically tuned dimensional augmentation as a versatile synthetic route towards robust metal-organic frameworks. *Nat. Comm.* (2014) DOI
8. R. L. Martin, **C. Simon**, B. Medasani, D. Britt, B. Smit, and M. Haranczyk. In silico Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species. *J. Phys. Chem. C*. (2014) DOI
7. R. L. Martin, **C. Simon**, B. Smit, M. Haranczyk. In silico design of porous polymer networks: high-throughput screening for methane storage materials. *J. Am. Chem. Soc.* (2014) DOI

6. **C. Simon**, J. Kim, L.C. Lin, R.L. Martin, M. Haranczyk, B. Smit. Optimizing nanoporous materials for gas storage. *PCCP*. (2014) DOI Front cover art.
5. R. L. Martin, H.C. Zhou, M.N. Shahrak, B. Smit, J. Swisher, **C. Simon**, J. Sculley, and M. Haranczyk. Modeling Methane Adsorption in Interpenetrating Porous Polymer Networks. *J. Phys. Chem. C*. (2013) DOI
4. **C. Simon**, I. Hepburn, W. Chen, E. De Schutter. The role of dendritic spine morphology in the compartmentalization and delivery of surface receptors. *J. Compt. Neurosci.* (2013) DOI
3. **C. Simon**, E. Vaughan, W. Bement, and L. Edelstein-Keshet. Pattern formation of Rho GTPases in single cell wound healing. *Mol. Biol. Cell*. (2013) DOI
2. K. Han, H. Hu, E. Ko, O. Ozer, **C. Simon**, C. Tan. A variational approach to modeling aircraft hoses and flexible conduits. *Mathematics-in-Industry Case Studies*. (2012) DOI
1. **C. Simon**, N. Yosinao. A mathematical model to distinguish the sociological and biological susceptibility factors in disease transmission in the context of H1N1/09 influenza. *J. Theor. Biol.* (2011) DOI

Recommended by Faculty of 1000

## Articles for public outreach

Personal blog: <http://corysimon.github.io/>

5. **C. Simon**, J. Kim, R. L. Martin, M. Haranczyk, B. Smit. Accelerating Materials Discovery with CUDA. *NVIDIA's Parallel for All blog*. (2015) Link
4. **C. Simon**, J. Kim, D. Gomez-Gualdrón, Y. Chung, R. L. Martin, R. Mercado, M. Deem, D. Gunter, M. Haranczyk, R. Snurr, and B. Smit. Computer-Aided Search for Materials to Store Natural Gas for Vehicles. *Frontiers for Young Minds*. (2015) Link
3. **C. Simon**. What are the best materials to separate a Xe/Kr mixture? *UC Berkeley ChemE Blog*. (2015) Link
2. **C. Simon** and B. Smit. Viagra ads and NSA watchlists: smoke but usually no fire. *Scientific American Guest Blog*. (2013) Link
1. **C. Simon**. Post-combustion CO<sub>2</sub> capture to mitigate climate change: separation costs energy. *Scientific American Guest Blog*. (2013) Link

## Professional experience

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|---------------------|---|
| 2017                | <b>Fellow</b> , <i>Altius Institute for Biomedical Sciences</i> , Seattle, Washington.<br>Developed statistical learning models to learn structure in enhancer-responsive gene promoters  |
| Summer 2016         | <b>Visiting Scholar</b> , <i>École Polytechnique Fédérale de Lausanne (EPFL)</i> , Sion, Switzerland.<br>Developed statistical mechanical model of porous crystals with rotating ligands  |
| Spring, Summer 2015 | <b>Department of Energy Fellow</b> , <i>Lawrence Berkeley National Lab</i> , Berkeley, CA.<br>Rapidly screened large databases of nanoporous materials using machine learning   |
| Fall 2014           | <b>Data Science Intern</b> , <i>Stitch Fix</i> , San Francisco, CA.<br>Developed and wrote recommendation algorithms for clothing purchases <ul style="list-style-type: none"> <li>○ Collaborative filtering</li> <li>○ Matrix factorization</li> <li>○ Software engineering in Python</li> <li>○ Working with data: SQL, Pandas</li> </ul> |
| Summer 2012         | <b>Research Intern</b> , <i>Okinawa Institute of Science and Technology</i> , Okinawa, Japan.<br>Investigated how the morphology of dendritic spines influences the compartmentalization of diffusing surface receptors using mathematical models   |
| Summer 2009         | <b>REU student</b> , <i>Virginia Bioinformatics Institute</i> , Blacksburg, VA.<br>Distinguished between sociological and biological factors in the transmission of H1N1/09 influenza using mathematical model  |
| 2007–2009           | <b>Chemical Engineering Co-op</b> , <i>Bridgestone Center for Research and Technology</i> , Akron, OH.<br>Characterized reaction rates in a bulk polymerization process to produce butadiene, wrote control programs in DeltaV  |
| Summer 2006         | <b>Research Assistant</b> , <i>Dept. of Chemical and Biomolecular Engineering</i> , Akron, OH.<br>Investigated the effect of wavelength of light on cyanobacteria growth  |

## Teaching experience

Outstanding Graduate Student Instructor Award at UC Berkeley, 2012.

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| Fall 2015 | <b>Graduate student instructor</b> , <i>Graduate Statistical Mechanics</i> , UC Berkeley.<br>Teaching effectiveness: 4.2/5.0 |
| Fall 2013 | <b>Graduate student instructor</b> , <i>Graduate Statistical Mechanics</i> , UC Berkeley.<br>Teaching effectiveness: 4.6/5.0 |

- Fall 2012 **Graduate student instructor**, *Material and Energy Balances*, UC Berkeley.  
Teaching effectiveness: 6.6/7.0
- Spring 2011 **Teaching assistant**, *Linear Systems*, University of British Columbia.  
Held computer lab session (programming in MATLAB)
- 2010-2012 **Math center drop-in tutor**, University of British Columbia.  
Spontaneously explained math problems to undergraduates using a dry erase board
- 2006, 2010 **Math and chemistry tutor**, University of Akron.

## Software

Github username: CorySimon

- pylAST: Python package for Ideal Adsorbed Solution Theory
- PEGrid: Julia package for analyzing potential energy of adsorbed molecules in nanoporous crystals

## Computer programming languages

Proficient scientific programmer (7 years, daily).

Python (numpy, scipy, pandas, scikit-learn), Julia, C, C++, CUDA, Bash, SQL.

Data visualization: Matplotlib, Seaborn, VisIt, Gadgetry.

## Workshops

- Aug 2011 **Mathematical Modeling in Industry**, *Institute for Mathematics and its Applications*, University of Minnesota, Minneapolis, MN.  
Modeled aircraft hoses and flexible conduits using calculus of variations. Mentored by Boeing mathematician, Thomas Grandine.

## Awards

- 2014 **DOE Office of Science Graduate Fellowship (SCGSR)**, *Lawrence Berkeley National Lab*.
- 2012 **Outstanding Graduate Student Instructor Award**, *UC Berkeley*.
- 2011-2013 **Pacific Institute of Mathematical Sciences Math Biology Fellowship**, *University of British Columbia*.
- 2010 **Department of Chemical Engineering Faculty Award**, *The University of Akron*.
- 2008, 2009 **The American Chemical Society (ACS) Rubber Division Scholarship**, *The University of Akron*.
- 2009 **Larry G. Foght Chemical Engineering Department Award**, *The University of Akron*.
- 2009, 2010 **Lubrizol Scholarship**, *The University of Akron*.
- 2006-2009 **Presidential Scholarship**, *The University of Akron*.
- 2006-2009 **Honors College Scholarship**, *The University of Akron*.

## Personal interests

Snowboarding, running, hiking, backpacking, snorkeling, playing guitar, traveling