CorySimon

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website
simonensemble.github.io

languages
Julia, Python

academic position

Assistant Professor (2017–present)
School of Chemical, Biological, and Environmental Engineering
Oregon State University

research group elevator pitch

We leverage machine learning, statistical mechanics, mathematical modeling, and molecular simulations to accelerate the discovery and deployment of nano-porous materials for gas storage, separations, and sensing.

education

2012–2016 **Ph.D.** in Chemical Engineering — University of California, Berkeley
Advisor: Berend Smit. GPA: 3.7/4.0.

2010–2012 ~~**Ph.D.**~~ in Mathematics (half-completed) — University of British Columbia
Advisor: Leah Keshet. Passed qualifying exams. Course average: 93.6%.

2005–2010 **B.S.** in Chemical Engineering — The University of Akron
Minor: Applied Mathematics
Summa Cum Laude. GPA: 3.993/4.0

experience

2017 **Altius Institute for Biomedical Sciences** — Seattle, WA.
Fellow
statistical machine learning models (ConvNets) to predict transcription-driving capacity of gene promoters

2016 **École Polytechnique Fédérale de Lausanne (EPFL)** — Sion, Switzerland
Visiting Scholar
statistical mechanical model of gas adsorption in porous crystals with rotating ligands

2015 **Lawrence Berkeley National Lab** — Berkeley, CA
US Department of Energy Fellow
random forests to screen large databases of nanoporous materials for gas separations

2014 **Stitch Fix** — San Francisco, CA
Data Science Intern
recommendation algorithms for clothing purchases (collaborative filtering, matrix factorization)

2012 **Okinawa Institute of Science and Technology** — Okinawa, Japan
Research Intern
mathematical models to understand how the morphology of dendritic spines influences the compartmentalization of diffusing surface receptors

2012 **Virginia Tech (Virginia Bioinformatics Institute)** — Blacksburgh, VA
REU student
age-structured mathematical models for the transmission of H1N1/09 influenza

2007–2009 **Bridgestone Center for Research and Technology** — Akron, OH
Chemical Engineering Co-op
development of bulk polymerization process for polybutadiene wrote control scheme programs in DeltaV

publications

Google Scholar Profile: 1426 citations, h-index 18, i10-index 22.

31. "An upper bound to gas storage and delivery via pressure-swing adsorption in porous materials." J. Pommerenck, C. Simon, D. Roundy. *arXiv*. (2020) DOI
30. "Message passing neural networks for partial charge assignment to metal-organic frameworks." A. Raza, A. Sturluson, C. Simon, X. Fern. *Journal of Physical Chemistry C*. (2020) DOI
29. "The SIR dynamic model of infectious disease transmission and its analogy with chemical kinetics." C. Simon. *ChemRxiv.* (2020) DOI
28. "Statistical thermodynamic model of gas adsorption in a metal-organic framework harboring a rotaxane molecular shuttle." J. Carney, D. Roundy, C. Simon. *ChemRxiv.* (2019) DOI
27. "Curating metal-organic frameworks to compose robust gas sensor arrays in dilute conditions." A. Sturluson, R. Sousa, Y. Zhang, M. T. Huynh, C. Laird, A. H. York, C. Silsby, C. H. Chang, C. Simon. *ACS Applied Materials & Interfaces*. (2020) DOI OSU News story
26. "Understanding Gas Storage in Cuboctahedral Porous Coordination Cages." L. Gregory, E. Gosselin, B. Trump, A. H. York, A. Sturluson, C. Rowland, G. Yap, C. Brown, C. Simon, E. Bloch. *Journal of the American Chemical Society* (2019) DOI
25. "The Role of Molecular Modeling and Simulation in the Discovery and Deployment of Metal-Organic Frameworks for Gas Storage and Separation." A. Sturluson, M. T. Huynh, A. Kaija, C. Laird, S. Yoon, F. Hou, Z. Feng, C. Wilmer, Y. Colon, Y. Chung, D. Siderius, C. Simon. *Molecular Simulation*. (2019) DOI
24. "Eigencages: Learning a latent space of porous cage molecules." A. Sturluson, M. T. Huynh, A. H. York, C. Simon. *ACS Central Science*. (2018) DOI OSU News story
23. "Multi- and instabilities in gas partitioning between nanoporous materials and rubber balloons." C. Simon, C. Carraro. *Proceedings of the Royal Society A*. (2019) DOI
22. "Xenon Gas Separation and Storage using Metal Organic Frameworks." D. Banerjee, C. Simon, S. Elsaidi, M. Haranczyk, P. Thallapally. *Chem*. (2018) DOI
21. "High-Throughput Computational Screening of Multivariate Metal-Organic Frameworks (MTV-MOFs) for CO_2 Capture." S. Li, Y. Chung, C. Simon, R. Snurr. *The Journal of Physical Chemistry Letters*. (2018) DOI
20. "Statistical mechanical model of gas adsorption in porous crystals with dynamic moieties." C. Simon, E. Braun, C. Carraro, B. Smit. *Proceedings of the National Academy of Sciences*. (2017) DOI
19. "Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks." S. Elsaidi, M. Mohamed, C. Simon, E. Braun, T. Pham, K. Forrest, W. Xu, D. Banerjee, B. Space, M. Zaworotko, P. Thallapally. *Chemical Science*. (2017) DOI
18. "Adsorbate-induced lattice deformation in the IRMOF-74 series." S. Jawahery, C. Simon, E. Braun, M. Witman, D. Tiana, B. Vlaisavljevich, B. Smit. *Nature Communications*. (2017) DOI
17. "The Materials Genome in action: identifying the performance limits of physical hydrogen storage." A. Thornton, C. Simon, J. Kim, O. Kwon, K. Deeg, K. Konstas, S. Pas, M. Hill, D. Winkler, M. Haranczyk, B. Smit. *Chemistry of Materials*. (2017) DOI
16. "Noria, a highly Xe-selective Nanoporous Organic Solid." R. Patil, D. Banerjee, C. Simon, J. Atwood, P. Thallapally. *Chemistry: A European Journal*. (2016) DOI Frontispiece, Hot paper, Chemistry Views story
15. "Metal-Organic Framework with Optimal Adsorption, Separation, and Selectivity towards Xenon." D. Banerjee, C. Simon, A. Plonka, R. Motkuri, J. Liu, X. Chen, B. Smit, J. Parise, M. Haranczyk, P. Thallapally. *Nature Communications*. (2016) DOI LBL story, EPFL story, Research Gate story, Chemical & Engineering News story
14. "Impact of the strength and spatial distribution of adsorption sites on methane deliverable capacity in nanoporous materials." D. Gomez-Gualdron, C. Simon, W. Lassman, D. Chen, R. L. Martin, M. Haranczyk, O. K. Farha, B. Smit, R. Q. Snurr. *Chemical Engineering Science*. (2016) DOI

13. "pyIAST: Ideal Adsorbed Solution Theory (IAST) Python package." C. Simon, B. Smit, M. Haranczyk. *Computer Physics Communications*. (2016) DOI
12. "What Are the Best Materials To Separate a Xenon/Krypton Mixture?" C. Simon, R. Mercado, S. K. Schnell, B. Smit, and M. Haranczyk. *Chemistry of Materials*. (2015) DOI
11. "The Materials Genome in Action: Identifying the Performance Limits to Methane Storage." C. Simon, J. Kim, D. Gomez-Gualdron, J. Camp, Y. Chung, R. L. Martin, R. Mercado, M.W. Deem, D. Gunter, M. Haranczyk, D. Sholl, R. Snurr, B. Smit. *Energy & Environmental Science* (2015) DOI Inside front cover art. Chemistry World story, EPFL story
10. "In Silico Discovery of High Deliverable Capacity Metal-Organic Frameworks." Y. Bao, R. L. Martin, C. Simon, M. Haranczyk, B. Smit, and M.W. Deem. *Journal of Physical Chemistry C* (2014) DOI
9. "Kinetically tuned dimensional augmentation as a versatile synthetic route towards robust metal-organic frameworks." 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. *Nature Communications*. (2014) DOI
8. "In silico Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species." R. L. Martin, C. Simon, B. Medasani, D. Britt, B. Smit, and M. Haranczyk. *Journal of Physical Chemistry C* (2014) DOI
7. "In silico design of porous polymer networks: high-throughput screening for methane storage materials." R. L. Martin, C. Simon, B. Smit, M. Haranczyk. *Journal of the American Chemical Society*. (2014) DOI
6. "Optimizing nanoporous materials for gas storage." C. Simon, J. Kim, L.C. Lin, R.L. Martin, M. Haranczyk, B. Smit. *Physical Chemistry Chemical Physics.* (2014) DOI Front cover art.
5. "Modeling Methane Adsorption in Interpenetrating Porous Polymer Networks." R. L. Martin, H.C. Zhou, M.N. Shahrak, B. Smit, J. Swisher, C. Simon, J. Sculley, and M. Haranczyk. *Journal of Physical Chemistry C*. (2013) DOI
4. "The role of dendritic spine morphology in the compartmentalization and delivery of surface receptors." C. Simon, I. Hepburn, W. Chen, E. De Schutter. *Journal of Computational Neuroscience*. (2013) DOI
3. "Pattern formation of Rho GTPases in single cell wound healing." C. Simon, E. Vaughan, W. Bement, and L. Edelstein-Keshet. *Molecular Biology of the Cell.* (2013) DOI
2. "A variational approach to modeling aircraft hoses and flexible conduits." K. Han, H. Hu, E. Ko, O. Ozer, C. Simon, C. Tan. *Mathematics-in-Industry Case Studies*. (2012) DOI
1. "A mathematical model to distinguish the sociological and biological susceptibility factors in disease transmission in the context of H1N1/09 influenza." C. Simon, N. Yosinao. *Journal of Theoretical Biology*. (2011) DOI Recommended by Faculty of 1000

open-source software

- **Controlz.jl**: Julia package to explore concepts in process dynamics and control
- **PorousMaterials.jl**: Julia package for molecular simulation of gas adsorption in porous crystals
- **pyIAST**: Python package for predicting mixed-gas adsorption isotherms in a porous material from pure-component gas adsorption isotherms via Ideal Adsorbed Solution Theory (IAST)

courses taught

ChE 361 **Process dynamics and simulation**
student evaluations: instructor's contribution to the course was 5.6/6.0.

ChE 461 **Process control**
student evaluations: instructor's contribution to the course was 5.6/6.0.

ChE 599 **Introduction to data science for engineers**
student evaluations: instructor's contribution to the course was 5.8/6.0.

students mentored

PhD students: Arni Sturluson, Nick Gantzler, Adrian Henle

undergraduate students: Jonathan Carney, Melanie Huynh, Mira Khare, Grant McConachie, Rachel Sousa, Arthur Henry York, Caleb Laird, Carson Silsby

technical blog

see simonensemble.github.io/blog.