CorySimon

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e-mail
cory.simon@x.edu
x =oregonstate

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

39. "Computation-informed optimization of Ni(PyC) functionalization for noble gas separations". N. Gantzler, M.-B. Kim, A. Robinson, M. W. Terban, S. Ghose, R. E. Dinnebier, A. H. York, D. Tiana, C. M. Simon, P. K. Thallapally. *ChemRxiv*. (2021) DOI

38. "`PoreMatMod.jl`: Julia package for in silico post-synthetic modification of crystal structure models". E. Adrian Henle, N. Gantzler, P. K. Thallapally, X. Z. Fern, C. Simon. *Journal of Chemical Information and Modeling*. (2021) DOI ACS Editors Choice.

37. "Bayesian optimization of nanoporous materials". A. Deshwal, C. Simon, J. R. Doppa. *Molecular Systems Design & Engineering.*. (2021) DOI

36. "Identifying gas composition changes to which non-injective gas sensor arrays are unresponsive". N. Gantzler, A. Henle, P. Thallapally, X. Fern, C. Simon. *Journal of Physics: Condensed Matter*. (2021) DOI

35. "A Recommendation System to Predict Missing Adsorption Properties of Nanoporous Materials". A. Sturluson, A. Raza, G. McConachie, D. Siderius, X. Fern, C. Simon. *Chemistry of Materials*. (2021) DOI

34. "An upper bound to gas storage and delivery via pressure-swing adsorption in porous materials." J. Pommerenck, C. Simon, D. Roundy. *arXiv*. (2020) DOI

33. "Adsorbed xenon propellant storage: are nanoporous materials worth the weight?" M. T. Huynh, N. Gantzler, S. Hough, D. Roundy, P. K. Thallapally, C. M. Simon. *Materials Advances*. (2021) DOI

32. "Towards explainable message passing networks for predicting carbon dioxide adsorption in metal-organic frameworks". A. Raza, F. Waqar, A. Sturluson, C. Simon and X. Fern. *Machine Learning for Molecules Workshop at NeurIPS 2020*. (2020) DOI

31. "Evaluating the Fitness of Combinations of Adsorbents for Quantitative Gas Sensor Arrays". R. Sousa, C. Simon. *ACS Sensors*. (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. *Peer J Physical Chemistry.* (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. *Langmuir.* (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

technical blog

see simonensemble.github.io/blog.

open-source software

- **Controlz.jl**: Julia package to explore concepts in process dynamics and control
- **Xtals.jl**: Julia package to work with crystal structures
- **PoreMatMod.jl**: Julia package to modify crystal structures, operating as a find-and-replace tool
- **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)

teaching

ChE 361 **Chemical process dynamics and simulation**
enrollment: 137.
course as a whole was 5.6/6.0 (median student evaluation)
instructor's contribution to the course was 5.7/6.0 (median student evaluation)

ChE 461 **Process control**
enrollment: 132.
no numeric student evaluations, but some comments from students:
"Dr. Simon is the best instructor I've had at this school."
"The videos went extremely well for this class. I was very impressed with how smoothly it went. While I still prefer in person, this class did the best remotely of my classes this term."
"Everything about Dr. Simon's classes is amazing. This is true of remote and in-person."
"Dr. Simon is a very intelligent and caring individual. He was able to explain difficult topics with ease. I also really enjoy how much his mathematics background comes through in the lecture which (for me) makes things easier to understand. Dr. Simon is also very transparent in how he grades and what to expect and was very easy to reach via Slack."

ChE 599 **Introduction to data science for engineers**
enrollment: 25.
course as a whole was 5.9/6.0 (median student evaluation)
instructor's contribution to the course was 5.9/6.0 (median student evaluation)

current research group members

PhD students

- Nick Gantzler
- Adrian Henle

- Paul Morris
- Gbenga Fabusola

MS students

- Ping Yang

undergraduate students

- Melanie Huynh
- Faaiq Waqar [co-advised by X. Fern]
- Kendra Hunt
- Nikolas Achatz [co-advised by X. Fern]
- Tristan Gavin [co-advised by X. Fern]

graduated research group members

PhD students

- Arni Sturluson

MS students

- Mark Geringer [co-advised by M. Campbell]

undergraduate students

- Jonathan Carney [co-advised by D. Roundy; now PhD student at University of North Carolina at Chapel Hill]
- Mira Khare [now PhD student at University of California, Berkeley]
- Arthur Henry York [now PhD student at University of California, Irvine]
- Carson Silsby [now PhD student at University of Idaho]
- Rachel Sousa [now PhD student at University of California, Irvine]
- Caleb Laird [now Environmental Engineer at CDM Smith]
- Grant McConachie [now post-bac position at the Frederick National Lab]
- Jack Draney [now PhD student at Princeton]

university service

- graduate admissions committee
- web advisory committee
- peer teaching evaluation committee

invited talks

- 3/2018. "Computational screening of nanoporous materials for gas separations." Siluria Technologies.
- 11/2019. "Curating Metal-Organic Frameworks to Compose Robust Gas Sensor Arrays." University of Pittsburgh. (Department of Chemical and Petroleum Engineering seminar)
- 8/2020. "Message passing neural networks for partial charge assignment to metal-organic frameworks." Korean Institute of Chemical Engineers (KIChE) National Conference. Keynote speaker.
- 3/2021. "The role of machine learning in the search for nanoporous materials for storing and separating gases." University of South Dakota. (Artificial Intelligence Symposium.)
- 2/2021. "Curating metal-organic frameworks for robust gas sensor arrays." University of California, Berkeley. (Department of Chemical & Biomolecular Engineering seminar)

- 11/2021. “Curating metal-organic frameworks for robust gas sensor arrays.” Arizona State University (Chemical Engineering Seminar)
- 11/2021. “Accelerating the search for performant adsorbent materials using machine learning.” International Adsorption Society Webinar. link on YouTube