ARNI STURLUSON

Chemical Engineering PhD

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EDUCATION

Ph.D. in Chemical Engineering

Oregon State University

Sept 2016 – Dec 2020

Thesis title: Novel Approaches to Porous Material Discovery

B.Sc. in Chemistry

University of Iceland

Sept 2012 – June 2015

EXPERIENCE

Graduate Research/Teaching Assistant

Oregon State University

September 2016 – December 2020 Corvallis, OR, USA

Undergraduate Research Assistant

University of Iceland

June 2016 – August 2016 Reykjavik, Iceland

PUBLICATIONS

1. **A. Sturluson**, M.T. Huynh, A.H.P. York, and C.M. Simon, "Eigencages: Learning a Latent Space of Porous Cage Molecules," *ACS Central Science* **2018** *4* (12), 1663–1676
2. **A. Sturluson**, M.T. Huynh, A. Kaija, C. Laird, S. Yoon, F. Hou, Z. Feng, C.E. Wilmer, Y.J. Colón, Y. Chung, D. Siderius, and C.M. Simon, "The Role of Molecular Modeling & Simulation in the Discovery and Deployment of Metal-Organic Frameworks for Gas Storage and Separation," *Molecular Simulation* **2019** *45* (14-15), 1082–1121
3. **A. Sturluson**, R. Sousa, Y. Zhang, M.T. Huynh, C. Laird, A.H.P. York, C. Silsby, C-H. Chang, and C.M. Simon, "Curating Metal-Organic Frameworks to Compose Robust Gas Sensor Arrays in Dilute Conditions," *ACS Appl. Mater. Interfaces* **2020** *12* (5), 6546–6564
4. G. Lorzing, E. Gosselin, B. Trump, A.H.P. York, **A. Sturluson**, C. Rowland, G.P.A. Yap, C.M. Brown, C.M. Simon, and E.D. Bloch, "Understanding Gas Storage in Cuboctahedral Porous Coordination Cages," *J. Am. Chem. Soc.* **2019** *141* (30), 12128–12138
5. A. Raza, **A. Sturluson**, C.M. Simon, and X. Fern, "Message passing neural networks for partial charge assignment to metal–organic frameworks," *J. Phys. Chem. C* **2020** *124* (35), 19070-19082
6. A. Raza, F. Waqar, **A. Sturluson**, C.M. Simon, and X. Fern, "Towards Explainable Message Passing Networks for Predicting Carbon Dioxide Adsorption in Metal–Organic Frameworks" *arXiv preprint* **2020** *arXiv:2012.03723*

STRENGTHS

molecular modelling · data visualization · recommender systems · deep learning · sensing operations

Julia · Python · Keras · MATLAB · LaTeX · Linux

LANGUAGES

English	●●●●●
Icelandic	●●●●●
German	●●●○○
Danish	●●●○○

SOFTWARE

PorousMaterials.jl
Developed and Contributed

MEDIA COVERAGE

Research zeroing in on electronic nose for monitoring air quality, diagnosing disease

Oregon State's Year in Science

CONFERENCE PROCEEDINGS

Poster Presentations

1. **A. Sturluson**, M.T. Huynh, A.H.P. York, and C.M. Simon, "Eigencages: Learning a Latent Space of Porous Cage Molecules," **2019** Graduate Research Showcase, Corvallis, OR, USA
2. **A. Sturluson**, M.T. Huynh, A.H.P. York, and C.M. Simon, "Eigencages: Learning a Latent Space of Porous Cage Molecules," **2019** *American Chemical Society* - Northwest Regional Meeting (NORM), Portland, OR, USA
3. **A. Sturluson**, R. Sousa, Y. Zhang, M.T. Huynh, C. Laird, A.H.P. York, C. Silsby, C-H. Chang, and C.M. Simon, "Curating Metal–Organic Frameworks to Compose Robust Gas Sensor Arrays" **2019** *American Institute of Chemical Engineers* - AIChE Annual Conference, Orlando, FL, USA

Talks

1. **A. Sturluson**, G. McConachie, M.T. Huynh, M. Khare, X. Fern, D. Siderius, and C.M. Simon, "A Recommender System to Rank Covalent–Organic Frameworks among Adsorption Properties," **2020** *American Institute of Chemical Engineers* - Virtual AIChE Annual Meeting

WORKSHOPS

1. **OSG User School 2018, Madison, WI, USA** Involved workshop detailing the effectiveness of the Open Science Grid computational power for high-throughput computations.