HAJIM SCHOOL OF ENGINEERING & APPLIED SCIENCES
UNIVERSITY of ROCHESTER

# The Department of Chemical Engineering Presents

## Prof. Cory M. Simon

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*"The design of an electronic nose as the construction of a well-conditioned inverse problem"*

**Abstract:** A robust electronic nose has applications in the monitoring of industrial processes, air quality, human and plant health, food freshness, and public areas (for security).

Owing to their adsorption properties, nanoporous materials such as metal-organic frameworks (MOFs) are poised to serve as sensitive and selective recognition elements for an electronic nose. The structural and chemical tunability of MOFs gives a large number of possible combinations of diverse MOFs to constitute an electronic nose.

In this talk, we frame the prediction of the gas composition from the response of an array of MOFs, given a thermodynamic adsorption model, as an inverse problem. The performance of the array of MOFs as an electronic nose is dictated by the conditioning of the inverse problem or, if present, the directions in gas composition space to which the array is unresponsive. This framing enables the computational design of a MOF-based electronic nose.

## Wednesday September 7, 2022

## The Gowen Room, 10:30-11:30 am

**Bio:** Cory Simon is an assistant professor of chemical engineering at Oregon State University. He earned his PhD in Chemical Engineering from the University of California, Berkeley. His research group leverages machine learning, statistical mechanics, mathematical modeling, and molecular simulations to accelerate the discovery and deployment of nanoporous materials for gas storage, separations, and sensing.