CIRC
2023-2024 Symposium Series

UNIVERSITY of ROCHESTER

Machine Learning-Guided Discovery of Polymer Membranes for CO_2 Separation

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Designing polymer membranes with high gas permeability and selectivity remains a grand challenge for energy, the environment, and economic sustainability. Increasing both the selectivity and permeability is a difficult multi-task constrained design problem for polymer membranes due to the trade-off between these two properties. The complexity of chemical composition and morphology of polymers makes this problem especially hard to attack with trial-and-error or intuition-based strategies. In this study, we instead present a machine learning (ML)-driven genetic algorithm to tackle the design problem of polymer membranes for CO_2 separation from N_2 and O_2. Using literature data of permeability for three gases, CO_2 , N_2 , and O_2, we constructed multiple ML models using different fingerprinting featurization schemes to predict all three gas permeabilities as well as the CO_2/N_2 and CO_2/O_2 selectivity values. Then, we employed a genetic algorithm to design new polymers and evaluated their performance with respect to the Robeson upper bounds using our machine learning models. We were able to identify new polymer membranes that are promising for both CO_2/N_2 and CO_2/O_2 separations. The top discovered polymers are predicted to have high glass transition temperatures, Tg. Similarly, the pyridine functionality was found in ~20% of the predicted polymers. Both of these facts are well in line with currently accepted experimental wisdom for CO_2 based separations. The framework developed here can be used to design polymers for any application involving constrained optimization. Finally, we outlined the strengths and limitations of this approach, as well as the imminent challenges and opportunities with using machine learning guided data-driven inverse design of polymers.

Practical Python Environments: A Guide to Using Python on BlueHive

Tod Romo, PhD

Center for Integrated Research Computing

Python is considered to be one of the preeminent scientific programming languages right now, but understanding its variants and how to handle installing packages and pipelines can be pretty perplexing. This talk will cover using Python on BlueHive, along with some of the different ways you can set up your own Python environments so that you can install and manage the software you need.

Friday, November 17, 2023 11:30 am - 1:00 pm

Wegmans Hall 1400