

# Guiding membrane design and development by machine learning

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## **Abstract:**

Machine learning has been a popular tool in the discovery and development of new materials. With proper algorithms, different models may be built to analyze the complex systems, identify the key features and guide material synthesis. In this presentation, we will introduce some of our preliminary efforts in applying machine learning for the fabrication of better membranes. First, Gradient Boosted Tree Models were trained to understand the material design and fabrication principles of thin film nanocomposite membranes for reverse osmosis. Second, literature data on metal organic framework based mixed matrix membranes for CO<sub>2</sub> separation were collected and trained by Random Forest Models. Based on model guidance, suitable MOFs were synthesized and membranes showed excellent performances which match well with model prediction. Transfer learning was also applied to save the resources. Third, artificial neural network was applied to reveal the formation mechanisms of nanofiltration membranes. Thereafter, membranes with high ion selectivity and permeance that surpass literature work were fabricated based on model guidance.

**Keywords:** Membrane, machine learning, carbon capture, nanofiltration, selectivity