

MATERIALS ENGINEERING

SEMINAR

**“MOLECULAR AND ATOMIC FEATURIZATION METHODS FOR PREDICTIVE
MODEL DESIGN”**

By

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ABSTRACT

Materials and molecular sciences have been concerned with the way chemical and structural information is represented when passed to a model for a number of decades. This has resulted in a large variety of options when it comes to representing atomic systems. Therefore, it can be challenging to optimize the representation and resulting descriptors for a specific application. Methods for dimensionality reduction and feature selection have been developed to aid researchers in this area. This review discusses the history of the representations that have been proposed and how they have been applied, as well as a demonstration of how dimensionality reduction and feature selection can be utilized to optimize the inputs for a given model.

Date: Friday, January 7, 2022

Time: 2:00pm

Place: Discovery Learning Research Center (DLRC) Room 131 or WebEx link:

https://purdue.webex.com/meet/strachan?_ga=2.116695814.1424719606.1638503067-1592143690.1634912070



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