



# Environmental Engineering & Sciences

Department of Civil and Environmental Engineering  
CEE 595AG Seminar

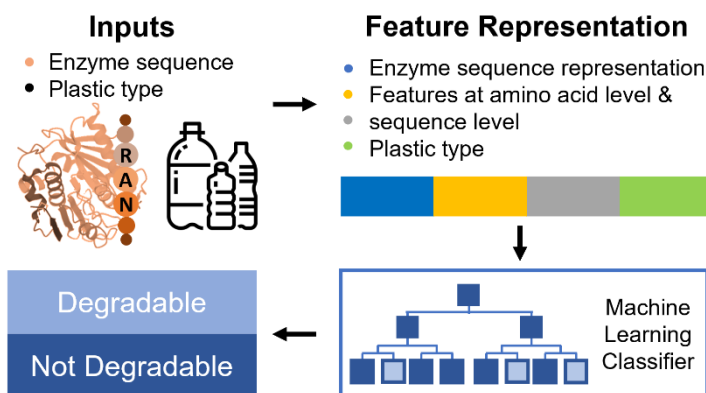
Friday, February 10, 2023 | 10:00 – 10:50 a.m. CST | 3310 Newmark Lab

## Machine Learning-Based Prediction of Enzymatic Degradation of Plastics Using Encoded Protein Sequence and Effective Feature Representation

Moderated by Yoonjoo Seo

Enzyme biocatalysis for plastic treatment and recycling is an emerging field of growing interest. However, it is challenging and time-consuming to identify plastic-degrading enzymes with desirable functionality given the large number of putative enzyme sequences. There is a critical need to develop an effective approach to accurately predict enzyme activity in degrading different types of plastics. In this study, we developed a machine learning-based Plastic Enzymatic Degradation (PED) framework to predict the ability of an enzyme to degrade plastics of interest by exploring and recognizing hidden patterns in protein sequences. A dataset integrating information from a wide range of experimentally verified enzymes and various common plastic substrates was created.

A new Context-aware Enzyme Sequence Representation (CESR) mechanism was developed to learn the abundant contextual information in enzyme sequences, and feature extraction was performed for enzymes at both amino acid level and protein sequence level. Thirteen machine learning classification algorithms were compared and XGBoost was identified as the best-performing algorithm. PED achieved an overall accuracy of 93.0% and outperformed sequence-based protein classification models from existing literature. Furthermore, important enzyme features in plastic degradation were identified and comprehensively interpreted. This study demonstrated a new tool for prediction and discovery of plastic-degrading enzymes.



### Renjing Jiang (Advisor Na Wei) PhD Student EES

Renjing is a 2nd year PhD student working with Dr. Na Wei in Environmental Engineering and Science. She got her Bachelor's degree in Environmental Engineering from Tongji University in China and her Master of Science at Stanford University. Her current research is on enzymatic degradation of plastics, where machine learning is used to identify hidden patterns from degradation data. Renjing is also interested in molecular and synthetic biology, and she plans to incorporate those technologies into her future research. In her spare time, she enjoys good food and Chinese Calligraphy.