

### **General Audience Abstract**

Plastics are often not readily degradable in the environment, and are thus fated to be pollutants. Because this is a problem we face, it is worthwhile to study how we can leverage computational power for the inverse design of polymers so that plastics can be preemptively designed to be more readily degradable and reduce their long term effect on the environment. Machine learning is a powerful technique of leveraging data and can be used as a tool for inversely designing polymers. Particularly, graph convolutional network (GCN) machine learning models are one way to make predictions about properties of polymers without the use of traditional complex hand-crafted information. Instead, they use graph representations of polymers to automatically learn task-specific representations through graph convolution techniques. However, the body of literature surrounding the application of the graph convolutional network to polymers is limited and often expresses doubt in the application of GCN models to polymers. But, in a recent paper, Prediction and Interpretation of Polymer Properties Using the Graph Convolutional Network, published by Park et al in 2022 provides evidence that GCN models can, in fact, be used reliably to predict properties of polymers. Thus, the purpose of this project is to recreate the Park study in order to affirm its findings and gain confidence in GCN machine learning models. Additionally, by means of recreating the Park study, a GCN model of similar accuracy was created, which grants the opportunity to improve it for better prediction accuracy. Knowing that GCNs are a reliable tool for predicting polymer properties allows us to apply it to the inverse design of polymers and even extend it to a more robust model with the capability to predict a multitude of properties that are pertinent to the degradability of plastics in the environment.