**Generating Novel Molecules Using Latent Dimension Reaction Manifolds from Deep Learning**

Project Sponsor: Pacific Northwest National Laboratory (PNNL)

Project Team: Christine Chang (Materials Science and Engineering), Liang Xu (Materials Science and Engineering), Chih-Wei Hsu (Chemical Engineering)

Abstract:

The vast majority of small organic molecules have yet to be identified, many of which are constituents of biofuels and biofuel crops. Deep learning can be used to both predict molecular properties and help identify novel molecular structures, which can subsequently be related to fuel properties and metabolic pathways. In this project sponsored by PNNL, we use variational autoencoders (VAEs) to encode known chemical reactions and build up a model that can search the latent space created by an already trained VAEs for candidate molecular structures. Our goal is to determine how chemical transformations are represented in latent space and to use latent space to predict products and product properties of chemical reactions.