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

Project Sponsor: Pacific Northwest National Laboratory (PNNL)

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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) in Darkchem, a package designed by PNNL, 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. One of the objective of this project is to determine the robustness of chemical reaction encoding in VAEs latent space and automate molecular structure generation from the latent space dimensions. If the latent space encoding of known reactions is found to be robust, we then can determine how chemical transformations are represented in latent space and to use latent space to predict products and product properties of chemical reactions. The results from this model have shown a very promising future for the usage of Darkchem to predict chemical reactions.