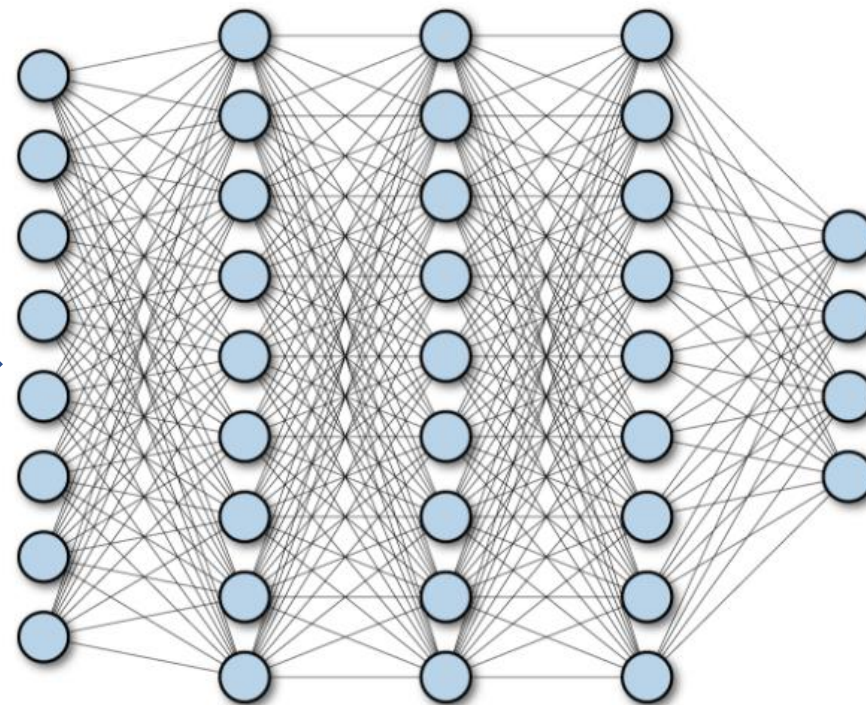# Artificial Neural Network Prediction

Smiles

RDKIT

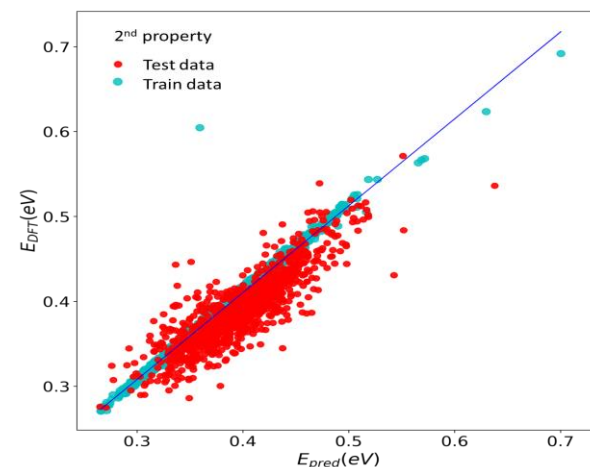2048 Fingerprints
from each molecule

Fully connected neural
network architecture

Loss Function - Mean absolute error

Optimizer - Adam

Submission 2: MLP's and Gaussian Process Regressors

For property 1,2,and 4, we trained individual fully connected MLP's using the same approach as described before.

We also trained a Gaussian Process Regressor to predict property 3 with a standard RBF Kernel and using a maximum likelihood loss function. On our validation set, we obtained a RMSD of 0.12 between the predicted and actual properties.

Other approaches:
- Autoencoders for dimensionality reduction.
- Pre-clustering the points based on Tanimoto similarity.