

Running Instructions:

Random_Forest.ipynb : this file contains training of Random Forest Algorithm for HOMO propertie.

Simple_NN.ipynb: this file contains training of simple neural network for HOMO propertie.

GNN_only.ipynb: this file contains training of GNN only model for HOMO propertie.

SOM_with_GNN.ipynb: this file contains training of GNN with SOM model for HOMO propertie.

MultipleProperties.ipynb: this file contains training of our main model SOM + GNN for four properties (alpha,HOMO,H,Cv) and stored trained model.

Pred_model.ipynb: this file can use for prediction using saved multiple properties SOM + GNN.

App.py: Contains code for Streamlit interface to predict four properties using SOM + GNN.

To run this file use command => `python -m streamlit run App.py`