Assignment#5

CH5650: Molecular Data Science and Informatic
Jan-May, 2025

Due Date: March 28, 2025 (Online Submission, https://courses.iitm.ac.in/)

Data: The position coordinates of all the atoms in a TiO2 crystal are given along with the forces acting on them. There is a total of 7815 configurations of TiO_2 crystals and their energy are provided. The data are in xsf (XCrysDen Structure File) format.

Problem Statement: Develop an ML model to predict the potential energy of TiO_2 based on the given data.