**What This Code Does:**

1. **Imports Required Libraries:**
   * **rdkit for chemical descriptor calculations.**
   * **torch for building and training a neural network.**
   * **matplotlib, numpy, pandas for data processing and visualization.**
2. **Defines Chemical Components:**
   * **Uses SMILES notation to represent Pigment (TiO₂), Extender (CaCO₃), and Binder (PVA).**
   * **Computes molecular descriptors (e.g., Molecular Weight, LogP, TPSA) using RDKit.**
3. **Loads Experimental Dataset:**
   * **Contains Pigment, Extender, Binder amounts and their corresponding Viscosity, Density, and pH values.**
4. **Feature Engineering:**
   * **Generates new chemical features by combining molecular descriptors and ingredient proportions.**
   * **Includes cross-component interactions to improve prediction accuracy.**
5. **Data Preprocessing:**
   * **Splits dataset into training (80%) and test (20%) sets.**
   * **Normalizes features using StandardScaler.**
   * **Converts data into PyTorch tensors for model training.**
6. **Builds a Neural Network:**
   * **4-layer architecture: Input → 32 neurons (ReLU) → 16 neurons (ReLU) → 8 neurons (ReLU) → Output (3 neurons for Viscosity, Density, pH).**
   * **Uses Dropout (0.3) to prevent overfitting.**
   * **Optimized with Adam optimizer & MSE loss.**
7. **Trains the Model:**
   * **Runs for up to 5000 epochs, with early stopping if validation loss doesn’t improve for 100 epochs.**
8. **Evaluates & Visualizes Results:**
   * **Plots training vs validation loss.**
   * **Compares actual vs predicted values for each target property.**
9. **Feature Importance Analysis:**
   * **Uses permutation importance to determine which features impact predictions the most.**
10. **Predicts Properties for New Data:**

* **Uses the trained model to predict Viscosity, Density, and pH for new formulations.**