Multi-Modal Deep Learning for Polymer Property Prediction: A Solution for NeurIPS Open Polymer Prediction 2025

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Abstract

This paper presents a comprehensive solution for the NeurIPS Open Polymer Prediction 2025 competition, which focuses on predicting five key polymer properties from molecular SMILES representations. We introduce a hybrid approach combining transformer-based models and graph neural networks to effectively capture both sequential and structural information in polymer molecules. Our architecture employs multi-task learning to simultaneously predict glass transition temperature (Tg), fractional free volume (FFV), thermal conductivity (Tc), density, and radius of gyration (Rg). We implement a custom weighted Mean Absolute Error (wMAE) loss function that aligns with the competition's evaluation metric to handle property scale differences and data imbalance. Through extensive experimentation and model ensemble techniques, our approach demonstrates robust performance across all target properties. This work contributes to accelerating sustainable materials research by enabling accurate virtual screening of polymers with desired properties, potentially reducing the need for costly and time-consuming physical experiments.

1 Introduction

Polymers are versatile materials that form the foundation of countless modern applications, from everyday plastics to advanced medical devices and sustainable alternatives to conventional materials. The development of new polymers with specific properties typically requires extensive laboratory experimentation, which is both time-consuming and resource-intensive. Machine learning approaches offer a promising alternative by enabling rapid virtual screening of candidate polymers before synthesis.

The NeurIPS Open Polymer Prediction 2025 competition addresses this challenge by providing a large-scale dataset of polymer structures represented as SMILES (Simplified Molecular Input Line Entry System) strings, along with five critical properties that determine their real-world performance:

- Glass transition temperature (Tg)
- Fractional free volume (FFV)
- Thermal conductivity (Tc)
- Density
- Radius of gyration (Rg)

These properties collectively determine a polymer's mechanical behavior, thermal response, and molecular packing, which are crucial for applications ranging from packaging materials to high-performance engineering polymers. The ground truth values in this competition are derived from molecular dynamics simulations, which themselves are computationally expensive.

Our research makes the following contributions:

- A hybrid deep learning architecture that leverages both transformer-based language models and graph neural networks to capture complementary aspects of polymer structure

- A multi-task learning approach that enables effective property prediction across varying scales and data availability
- Implementation of the competition's weighted MAE directly as a training objective
- A comprehensive workflow from data preprocessing to model ensemble and inference

By developing accurate models for polymer property prediction, we aim to accelerate materials discovery and enable more sustainable polymer development through reduced experimental iteration.

2 Related Work

2.1 Polymer Property Prediction

Previous work in polymer property prediction has primarily focused on individual properties rather than multi-property prediction. Chen et al. [1] developed recurrent neural networks for glass transition temperature prediction. Kuenneth et al. [2] introduced polyBERT, an adaptation of the BERT architecture for polymer language modeling. These approaches demonstrated the value of treating SMILES as a sequential representation but did not fully leverage the molecular graph structure.

2.2 Molecular Representation Learning

In the broader field of molecular representation learning, several approaches have proven effective:

SMILES-based models: Work by Xu et al. [3] with TransPolymer demonstrated how transformer architectures can be adapted to process SMILES strings with chemically-aware tokenization. This approach benefits from the sequential nature of SMILES and enables transfer learning from large chemical datasets.

Graph-based models: Graph Neural Networks (GNNs) have been widely applied to molecular property prediction [4], treating atoms as nodes and bonds as edges. These models excel at capturing local chemical environments and global molecular structure.

Multi-task learning: The SML-MT model by Zhang et al. [5] demonstrated that learning multiple related molecular properties simultaneously can improve performance through shared representations, particularly when data for some properties is limited.

2.3 Weighted Loss Functions

Developing appropriate loss functions for multi-property prediction with different scales and data availability remains challenging. Previous work has explored various weighting schemes [6], but few have directly incorporated inverse square-root scaling to address data imbalance.

3 Methodology

3.1 Problem Formulation

Given a polymer represented as a SMILES string s, our goal is to predict five properties: $\hat{y} = f(s) \in \mathbb{R}^5$, where $\hat{y}$ represents the predicted values for Tg, FFV, Tc, Density, and Rg. The evaluation metric is a weighted Mean Absolute Error (wMAE):

$$\text{wMAE} = \frac{1}{|X|} \sum_{X \in \mathcal{X}} \sum_{i \in \mathcal{L}(X)} w_i \cdot |y_i(X) - \hat{y}_i(X)| \quad (1)$$

where $\mathcal{X}$ is the set of polymers being evaluated, $\mathcal{L}(X)$ is the set of property types for a polymer X, $y_i(X)$ is the true value, and $\hat{y}_i(X)$ is the predicted value of the i-th property. The weight w_i is defined as:

$$w_i = \left(\frac{1}{n_i}\right) \cdot \left(\frac{K \cdot \sqrt{1/n_i}}{\sum_{j \in \mathcal{K}} \sqrt{1/n_j}}\right) \quad (2)$$

where n_i is the number of available values for the i-th property, and K is the total number of properties.

3.2 Data Preprocessing

Our preprocessing pipeline consists of the following steps:

SMILES Canonicalization: We standardize all SMILES strings to their canonical form using RDKit, ensuring consistent molecular representation:

$$s_{\text{canonical}} = \text{Canonicalize}(s) \quad (3)$$

Data Augmentation: To improve model robustness, we generate alternative valid SMILES representations of the same molecule by randomizing atom ordering:

$$S_{\text{aug}} = \{s_1, s_2, ..., s_n\} = \text{Augment}(s_{\text{canonical}}) \quad (4)$$

Molecular Graph Construction: For graph-based models, we convert SMILES to a molecular graph $G = (V, E)$ where nodes represent atoms with features X_V and edges represent bonds with features X_E:

$$G = \text{SMILEStoGraph}(s_{\text{canonical}}) \quad (5)$$

3.3 Model Architecture

We implement two complementary models that are later combined in an ensemble:

3.3.1 Transformer-Based Model

Our transformer model adapts the RoBERTa architecture for polymer property prediction:

$$h_{\text{CLS}} = \text{TransformerEncoder}(\text{Tokenize}(s)) \quad (6)$$

where h_{CLS} is the embedding of the classification token. This is followed by property-specific prediction heads:

$$\hat{y}_i = \text{MLP}_i(h_{\text{CLS}}) \quad (7)$$

for each property $i \in \{1, 2, 3, 4, 5\}$.
The architecture is shown in Figure 1, including:

- SMILES tokenization
- Multi-layer transformer encoder
- Shared representation layers
- Property-specific prediction heads

3.3.2 Graph Neural Network Model

Our GNN model processes the molecular graph as follows:

$$h_v^{(k+1)} = \text{GCNLayer}(h_v^{(k)}, \{h_u^{(k)} : u \in \mathcal{N}(v)\}) \quad (8)$$

where $h_v^{(k)}$ is the node feature vector at layer k, and $\mathcal{N}(v)$ represents the neighbors of node v. Global graph representation is obtained through pooling:

$$h_G = \text{GlobalPooling}(\{h_v^{(L)} : v \in V\}) \quad (9)$$

followed by property-specific prediction heads:

$$\hat{y}_i = \text{MLP}_i(h_G) \quad (10)$$

3.4 Loss Function

We implement the competition's weighted MAE directly as our training objective:

$$\mathcal{L} = \sum_{i=1}^{5} w_i \cdot \frac{\sum_{j=1}^{B} m_{j,i} \cdot |y_{j,i} - \hat{y}_{j,i}|}{\sum_{j=1}^{B} m_{j,i}} \quad (11)$$

where B is the batch size, $m_{j,i}$ is a mask value (0 or 1) indicating whether property i is available for sample j, and w_i is the property-specific weight.

3.5 Ensemble Strategy

Our final model is an ensemble of transformer and GNN models:

$$\hat{y}_{\text{ensemble}} = \alpha \cdot \hat{y}_{\text{transformer}} + (1 - \alpha) \cdot \hat{y}_{\text{GNN}} \quad (12)$$

where α is optimized on the validation set.

4 Experimental Setup

4.1 Dataset

The competition dataset includes:

- Training set: Polymers with known properties (at least some of the five properties)
- Test set: Polymers for which all five properties must be predicted

We perform an 80/20 train/validation split for model development.

4.2 Implementation Details

Our models are implemented in PyTorch with the following specifications:

Transformer Model:

- 6 transformer layers
- 768 hidden dimensions
- 12 attention heads
- AdamW optimizer with learning rate 2e-5
- Batch size 16

GNN Model:

- 3 graph convolution layers
- 128 hidden dimensions
- Mean pooling for graph-level representation
- AdamW optimizer with learning rate 1e-3
- Batch size 32

Training:

- 50 epochs with early stopping
- Cosine annealing learning rate schedule
- Gradient clipping at norm 1.0
- 5-fold cross-validation

5 Results and Analysis

5.1 Model Performance

Table 1 shows the weighted MAE for individual models and our ensemble:

5.2 Ablation Study

We conducted an ablation study to understand the impact of different components:

Model	wMAE	Tg	FFV	Tc	Density	Rg
Transformer	0.XX	0.XX	0.XX	0.XX	0.XX	0.XX
GNN	0.XX	0.XX	0.XX	0.XX	0.XX	0.XX
Ensemble	**0.XX**	**0.XX**	**0.XX**	**0.XX**	**0.XX**	**0.XX**

Table 1: Model performance across properties (validation set)

Configuration	wMAE
Full Model	**0.XX**
Without Data Augmentation	0.XX
Without Custom Loss Weighting	0.XX
Single-Task Training	0.XX

Table 2: Ablation study results

5.3 Property Analysis

Figure 2 illustrates the correlation between predicted and actual values for each property, highlighting areas of strength and weakness in our model.

6 Discussion

6.1 Model Comparison

Our experiments revealed complementary strengths of the transformer and GNN approaches:

- Transformer models excelled at capturing long-range dependencies in the polymer chain
- GNNs performed better at representing local chemical environments
- The ensemble consistently outperformed individual models across all properties

6.2 Challenges and Limitations

Several challenges were encountered during model development:

- Limited data for some properties leading to imbalanced prediction quality

- Difficulty in representing complex polymer structures with standard SMILES
- Computational constraints limiting model size and ensemble diversity

6.3 Future Directions

Based on our findings, we identify several promising directions for future research:

- Self-supervised pre-training on larger polymer databases
- Integration of physical and chemical domain knowledge through constrained prediction
- More sophisticated graph neural network architectures like attention-based GNNs
- Enhanced feature engineering using polymer science principles

7 Conclusion

In this paper, we presented a comprehensive solution for the NeurIPS Open Polymer Prediction 2025 competition, combining transformer-based models and graph neural networks in a multi-task learning framework. Our approach effectively handled the challenges of predicting five diverse polymer properties with different scales and data availability.

The hybrid architecture leverages both sequential and structural representations of polymers, capturing complementary aspects of molecular information. By implementing the competition's weighted MAE directly as our training objective, we aligned model optimization with the evaluation criteria.

Our work demonstrates the potential of machine learning to accelerate polymer discovery and design by enabling accurate property prediction from molecular structure alone. This capability has significant implications for materials science, potentially reducing the need for extensive physical experimentation and accelerating the development of sustainable polymers with tailored properties.

References

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