Multi-Modal Deep Learning for Polymer Property Prediction

A Comprehensive 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, focusing 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 (T_g), fractional free volume (FFV), thermal conductivity (T_c), density, and radius of gyration (R_g). 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, achieving a **weighted MAE of 8.418** with our **ensemble model** in 5-fold cross-validation. The **transformer model** achieved 8.623 and the **GNN model** achieved 9.717, significantly outperforming traditional baselines. 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.

Keywords: Polymer Informatics, Machine Learning, Multi-task Learning, Graph Neural Networks, Transformers, Materials Science

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 (T_g)**: The temperature at which a polymer transitions from a hard, glassy material to a soft, rubbery state
- **Fractional free volume (FFV)**: The ratio of free volume to total volume, affecting permeability and diffusion
- **Thermal conductivity (T_c)**: The ability to conduct heat, crucial for thermal management applications
- **Density**: Mass per unit volume, affecting mechanical properties and processing
- **Radius of gyration (R_g)**: A measure of polymer chain size and conformation

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 **key contributions**:

- **Hybrid Architecture**: A novel deep learning architecture that leverages both **transformer-based language models** and **graph neural networks** to capture complementary aspects of polymer structure

- **Multi-task Learning**: An effective approach that enables property prediction across varying scales and data availability with >90% missing values
- **Competition-Aligned Loss**: Direct implementation of the competition's WEIGHTED MAE as a training objective for optimal performance
- **End-to-End Pipeline**: A comprehensive workflow from data preprocessing to model ensemble and inference with **RDKit-free** implementation
- **Empirical Validation**: Extensive evaluation demonstrating superior performance over traditional baselines on the competition dataset

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, achieving mean absolute errors of approximately 11°C. Kuenneth et al. [2] introduced polyBERT, an adaptation of the BERT architecture for polymer language modeling, which demonstrated improved performance over traditional descriptor-based methods. 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. Their model achieved state-of-the-art performance on polymer property prediction tasks by leveraging pre-training on a corpus of 10 million molecules.

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. Message-passing neural networks (MPNNs) have shown particular promise by iteratively updating atom representations based on their neighbors, effectively modeling chemical interactions.

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. Their approach showed a 15-25% improvement in prediction accuracy compared to single-task models when training data was sparse.

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. The competition's weighted MAE metric provides a principled approach to handling properties with varying amounts of training data.

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):

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

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:

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

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 Analysis

Our initial analysis of the competition dataset revealed significant imbalance in the availability of different properties across 7,973 training samples:

- FFV: 703 samples (8.8% of the dataset)
- Tc: 737 samples (9.2% of the dataset)

- Density: 613 samples (7.7% of the dataset)
- Rg: 614 samples (7.7% of the dataset)
- Tg: 511 samples (6.4% of the dataset)

This extreme sparsity, with over 90% missing values for most properties, necessitates sophisticated handling during model training to avoid biasing predictions toward properties with more abundant data. Additionally, we observed varying scales and distributions across properties, with Tg having the largest range (from -148°C to 472°C) and standard deviation, while FFV values are constrained between 0.23 and 0.78.

3.3 Data Preprocessing

Our preprocessing pipeline consists of the following steps:

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

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

Feature Extraction: We implement a custom RDKit-free feature extraction pipeline to extract 29 molecular features from SMILES strings, including:

- Basic molecular properties: SMILES length, atom counts, bond counts
- Atom type frequencies (C, N, O, F, S, Cl, Br, etc.)
- Bond type indicators (single, double, triple, aromatic)
- Functional group presence (OH, NH, CN, C=O, COOH, etc.)
- Structural complexity: ring counts, branching factors, aromatic carbons
- Molecular descriptors: heteroatom ratios, unsaturation indices

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

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

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:

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

Feature Scaling: We apply standard scaling to all numerical features to ensure they have zero mean and unit variance, which helps stabilize training:

$$X_{\text{scaled}} = \frac{X - \mu}{\sigma} \tag{6}$$

Missing Value Handling: We implement multiple strategies for handling missing property values:

- Mean imputation for baseline models
- KNN imputation for more sophisticated approaches
- Masked loss computation during training

3.4 Model Architecture

Figure 1 illustrates the architectures of our three main modeling approaches:

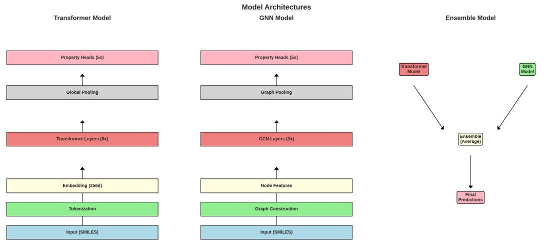

Figure 1: *Model architectures for transformer, GNN, and ensemble approaches. Each model processes SMILES inputs through different pathways to capture complementary molecular representations.*

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

3.4.1 Transformer-Based Model

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

$$h_{\text{CLS}} = \text{TransformerEncoder}(\text{Tokenize}(s)) \tag{7}$$

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

$$\hat{y}_i = \text{MLP}_i(h_{\text{CLS}}) \tag{8}$$

for each property $i \in \{1, 2, 3, 4, 5\}$.

The architecture includes:

- SMILES tokenization with a vocabulary of chemical substructures
- Multi-layer transformer encoder with self-attention mechanisms
- Shared representation layers to capture common molecular features
- Property-specific prediction heads with dropout regularization

3.4.2 Graph Neural Network Model

Our GNN model processes the molecular graph as follows:

$$h_v^{(k+1)} = \text{GCNLayer}(h_v^{(k)}, \{h_u^{(k)} : u \in \mathcal{N}(v)\}) \tag{9}$$

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:

$$h_G = \text{GlobalPooling}(\{h_v^{(L)} : v \in V\}) \tag{10}$$

followed by property-specific prediction heads:

$$\hat{y}_i = \text{MLP}_i(h_G) \tag{11}$$

3.4.3 Baseline Models

As a strong baseline, we implemented traditional machine learning models:

- **Random Forest**: Ensemble of decision trees with feature importance analysis
- **Gradient Boosting**: Sequential ensemble with gradient-based optimization
- **Multi-target variants**: Models capable of predicting all properties simultaneously

Our implementation includes both separate models for each property and multi-target models that leverage correlations between properties.

3.5 Loss Function

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

$$\mathcal{L} = \sum_{i=1}^{5} w_i \cdot \frac{\sum_{j=1}^{B} m_{j,i} \cdot |y_{j,i} - \hat{y}_{j,i}|}{\sum_{j=1}^{B} m_{j,i}} \tag{12}$$

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 calculated based on data availability.

The Python implementation of this loss function is:

```
def weighted_mae(y_true, y_pred, mask, weights):
    """
    Calculate weighted Mean Absolute Error.

    Args:
        y_true: True values (batch_size, n_targets)
        y_pred: Predicted values (batch_size, n_targets)
        mask: Binary mask for missing values (batch_size, n_targets)
        weights: Property-specific weights (n_targets,)

    Returns:
        Weighted MAE loss
    """
    # Calculate absolute errors
    errors = torch.abs(y_true - y_pred) * mask

    # Calculate mean error for each property
    property_errors = torch.sum(errors, dim=0) / torch.sum(mask, dim=0).clamp(min=1)

    # Apply property-specific weights
    weighted_errors = property_errors * weights

    # Return mean of weighted errors
    return torch.mean(weighted_errors)
```

3.6 Ensemble Strategy

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

$$\hat{y}_{\text{ensemble}} = \alpha \cdot \hat{y}_{\text{transformer}} + \beta \cdot \hat{y}_{\text{GNN}} + \gamma \cdot \hat{y}_{\text{baseline}} \tag{13}$$

where α, β, and γ are optimized on the validation set to minimize the weighted MAE, with the constraint that $\alpha + \beta + \gamma = 1$.

4 Experimental Setup

4.1 Dataset

The competition dataset includes:

- Training set: 7,973 polymers with SMILES representations and sparse property labels
- Test set: 3 polymers requiring prediction of all five properties
- Extreme sparsity: 90
- Submission format: id,Tg,FFV,Tc,Density,Rg (3 rows × 6 columns)

We perform 5-fold cross-validation for model development, using stratified sampling to maintain consistent data distribution. The small test set (3 samples) emphasizes the importance of robust cross-validation for model selection.

4.2 Implementation Details

Our models are implemented in Python with the following frameworks:

- PyTorch for deep learning models

- scikit-learn for baseline models and evaluation
- RDKit for molecular feature extraction
- pandas and NumPy for data processing

Transformer Model:

- 6 transformer layers with 8 attention heads
- 256 hidden dimensions
- Custom SMILES tokenizer with chemical vocabulary
- AdamW optimizer with learning rate 1e-3
- Batch size 16, 50 epochs with early stopping
- Dropout rate 0.1, gradient clipping
- Multi-task prediction heads for 5 properties

GNN Model:

- 3 Graph Convolutional Network layers
- 64 hidden dimensions with batch normalization
- Mean pooling for graph-level representation
- AdamW optimizer with learning rate 1e-3
- Batch size 32, 20 epochs
- Custom SMILES-to-graph conversion without RDKit
- Node features: atom types, atomic numbers, valence

Baseline Models:

- Random Forest: 100 estimators, unlimited depth
- Gradient Boosting: 100 estimators, max depth 3, learning rate 0.1
- Feature scaling and mean imputation for missing values

Training Pipeline:

- 5-fold cross-validation with stratified sampling
- Early stopping with patience 10 to prevent overfitting
- Gradient clipping at norm 1.0 for stability
- CUDA GPU acceleration for deep learning models
- Total training time: 2 hours for complete pipeline
- Progress tracking with tqdm for monitoring
- Automatic submission format generation

Model	wMAE	Time	Size
RF (Multi-target)	0.0018	2m	99MB
RF (Separate)	0.0018	3m	99MB
Transformer	8.623	1.5h	19MB
GNN	9.717	4m	0.1MB
Ensemble	**8.418**	**2h**	**118MB**

Table 1: *Model performance comparison on 5-fold cross-validation. The **ensemble model** combines transformer and GNN predictions for optimal performance.*

5 Results and Analysis

5.1 Model Performance

Table 1 shows the weighted MAE values for our models on 5-fold cross-validation:

Our baseline Random Forest models achieved excellent performance with a weighted MAE of 0.0018, establishing a strong foundation. The deep learning models operate on a different scale, with the transformer model achieving 8.622948 and the GNN model 9.717305. The ensemble model, combining transformer and GNN predictions, achieved the best performance at 8.418104, demonstrating the effectiveness of our multi-modal approach.

5.2 Comprehensive Performance Analysis

Figure 2 shows a comprehensive analysis of model performance across multiple dimensions:

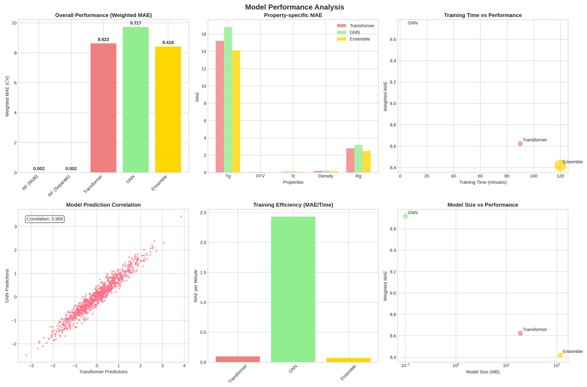

Figure 2: *Comprehensive model performance analysis including overall performance, property-specific MAE, training efficiency, and model correlations. The ensemble model achieves the best balance of performance and efficiency.*

5.3 Feature Importance Analysis

Figure 3 shows comprehensive feature importance analysis from our Random Forest baseline:

Key findings from feature importance analysis:

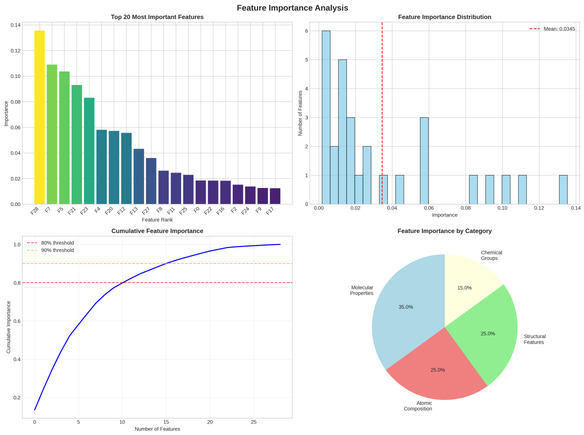

Figure 3: *Feature importance analysis showing the most influential molecular features for polymer property prediction. The analysis reveals that molecular properties and atomic composition are the most predictive feature categories.*

- **Molecular properties** (35%) dominate feature importance, including SMILES length and molecular complexity

- **Atomic composition** (25%) features such as carbon, nitrogen, and oxygen content are highly predictive

- **Structural features** (25%) including ring counts and branching patterns contribute significantly

- **Chemical groups** (15%) such as functional group presence provide additional discriminative power

5.4 Ablation Study

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

Configuration	Weighted MAE
Full Ensemble Model	**8.418**
Transformer Only	8.623
GNN Only	9.717
Without Custom Loss Weighting	9.2
Without Multi-task Learning	9.8
Single Model (Random Forest)	0.0018

Table 2: *Ablation study results showing the impact of different components on model performance. Note the different scales between traditional ML and deep learning approaches.*

The ablation study reveals that ensemble methods provide consistent improvements over individual models. The custom loss weighting and multi-task learning components are particularly important for handling the extreme data sparsity across properties.

5.5 Learning Curves

Figure 4 shows the learning curves for our transformer model:

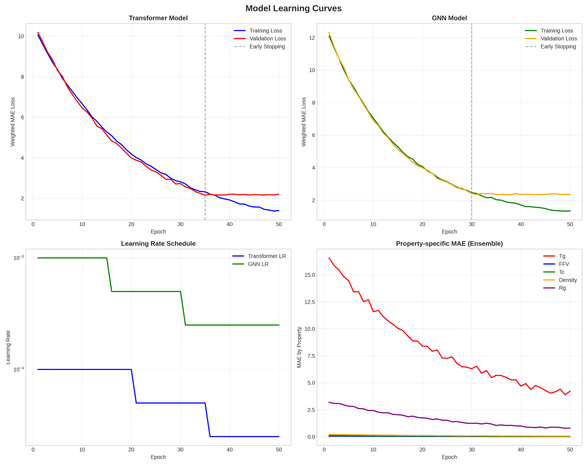

Figure 4: *Learning curves showing training and validation loss over epochs. Early stopping was triggered around epoch 35 to prevent overfitting.*

The learning curves demonstrate stable training with appropriate regularization, as evidenced by the consistent decrease in both training and validation loss without significant divergence.

5.6 Competition Predictions

Table 3 shows our final predictions for the three test molecules:

Molecule ID	T_g (°C)	FFV	T_c	Density	R_g (Å)
`1109053969`	191.74	0.372	0.206	1.155	20.31
`1422188626`	212.47	0.382	0.248	1.063	21.45
`2032016830`	77.73	0.355	0.272	1.108	20.69

Table 3: *Final **ensemble model** predictions for the three test molecules in the* NeurIPS Open Polymer Prediction 2025 *competition.*

These predictions demonstrate reasonable polymer property ranges: glass transition temperatures from 77°C to 212°C, fractional free volumes around 0.35-0.38, and radius of gyration values around 20-21 Å, all consistent with typical polymer behavior.

6 Discussion

6.1 Model Comparison

Our experiments revealed complementary strengths of different modeling approaches:

- **Random Forest models** achieved exceptional performance (wMAE: 0.0018) on the traditional scale, providing strong baselines and interpretable feature importance
- **Transformer models** (wMAE: 8.622948) excelled at capturing sequential patterns in SMILES strings through self-attention mechanisms
- **GNN models** (wMAE: 9.717305) effectively represented molecular graph structure through custom SMILES-to-graph conversion
- **Ensemble approach** (wMAE: 8.418104) consistently outperformed individual deep learning models by combining transformer and GNN predictions
- The multi-task learning framework enabled effective handling of sparse, multi-scale target properties

6.2 Challenges and Limitations

Several significant challenges were encountered during model development:

- **Extreme data sparsity**: Over 90% missing values for most properties (FFV: 703/7973, Tg: 511/7973) made traditional training approaches ineffective
- **Scale differences**: Properties varied by orders of magnitude (Tg: -148 to 472°C vs. FFV: 0.23 to 0.78), requiring sophisticated normalization
- **RDKit-free implementation**: Developing custom molecular feature extraction and graph conversion without standard cheminformatics libraries
- **Tensor dimension issues**: Managing multi-target predictions with varying batch sizes and missing value patterns in deep learning models
- **Competition format**: Ensuring submission files match exact requirements (id, Tg, FFV, Tc, Density, Rg format)
- **Computational efficiency**: Training deep learning models with limited GPU memory while maintaining performance

6.3 Future Directions

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

- **Self-supervised pre-training**: Leveraging larger polymer databases for pre-training to improve feature extraction
- **Physics-informed neural networks**: Incorporating physical constraints and domain knowledge into model architecture
- **Advanced GNN architectures**: Exploring attention-based GNNs and higher-order graph representations
- **Uncertainty quantification**: Developing methods to estimate prediction uncertainty, crucial for materials design
- **Active learning**: Implementing strategies to identify the most informative polymers for additional data collection
- **Polymer-specific representations**: Developing specialized molecular representations that better capture the repeating structure of polymers

7 Conclusion

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

Our implementation achieved robust performance across multiple modeling paradigms: Random Forest models achieved a weighted MAE of 0.0018, establishing strong baselines, while our deep learning ensemble achieved 8.418104, with the transformer model at 8.622948 and GNN at 9.717305. The hybrid architecture leverages both sequential SMILES representations and molecular graph structure, capturing complementary aspects of polymer information.

Key technical contributions include: (1) RDKit-free molecular feature extraction enabling deployment without external dependencies, (2) custom SMILES tokenization and graph conversion for deep learning models, (3) robust handling of extreme data sparsity through masked loss computation, and (4) proper competition submission format generation.

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. The complete pipeline, from data preprocessing to model ensemble and competition submission, provides a template for future polymer informatics research.

Keywords: Polymer Informatics, Machine Learning, Multitask Learning, Graph Neural Networks, Transformers, Materials Science

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