33rd ACM International Conference on Information and Knowledge Management
October 21-25, 2024

MMPolymer: A Multimodal Multitask Pretraining Framework for Polymer Property Prediction

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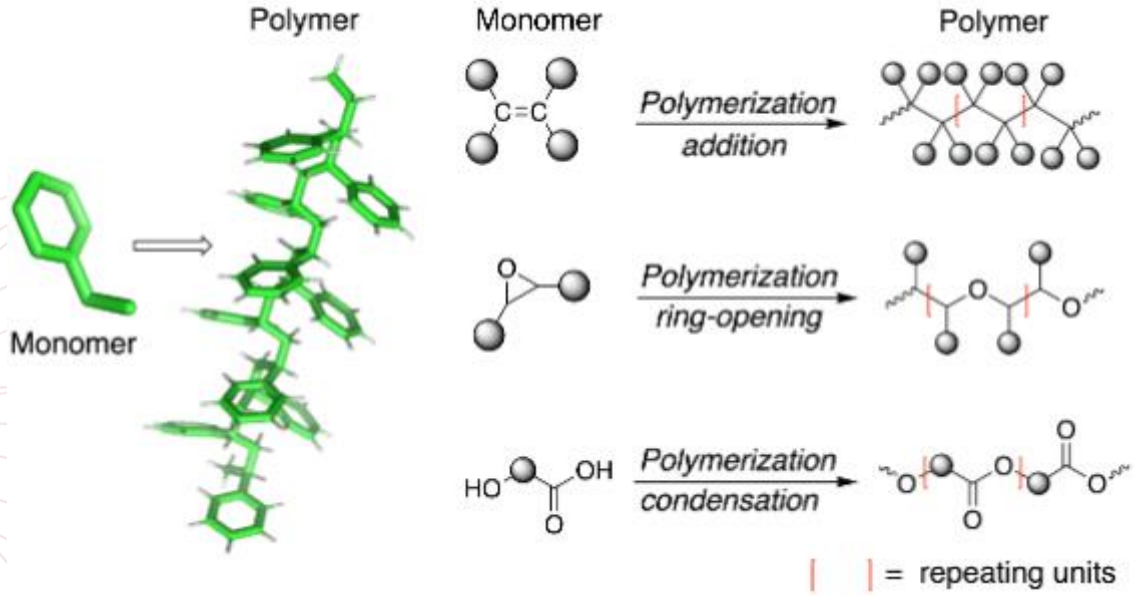
October 22, 2024

Background

■ Polymer

- **Polymers** are **high-molecular-weight compounds** constructed by the covalent bonding of numerous identical or similar **monomers**.
- In the past few decades, they have played an **important role** in many scientific fields, such as chemistry, material science, and drug design.



Background

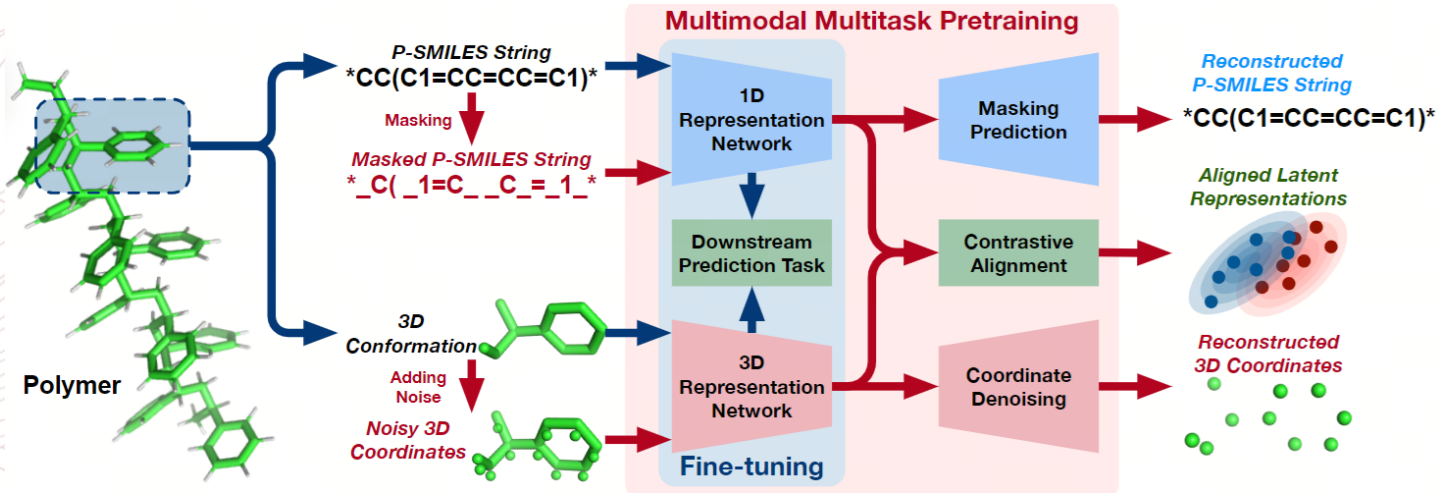
■ Polymer Property Prediction

- In this case, achieving accurate **prediction of polymer properties** has garnered more and more attention due to its significance:
  - Predicting polymer properties like plasticity and conductivity helps guide the design and development of polymer-based materials.
  - Predicting polymeric drug carriers' bio-compatibility and release kinetics is essential for designing effective and safe drugs.
  - …
- However, existing prediction methods heavily rely on the information learned from polymer SMILES sequences (**P-SMILES** strings) while ignoring 3D structural information, leading to sub-optimal performance.

Background

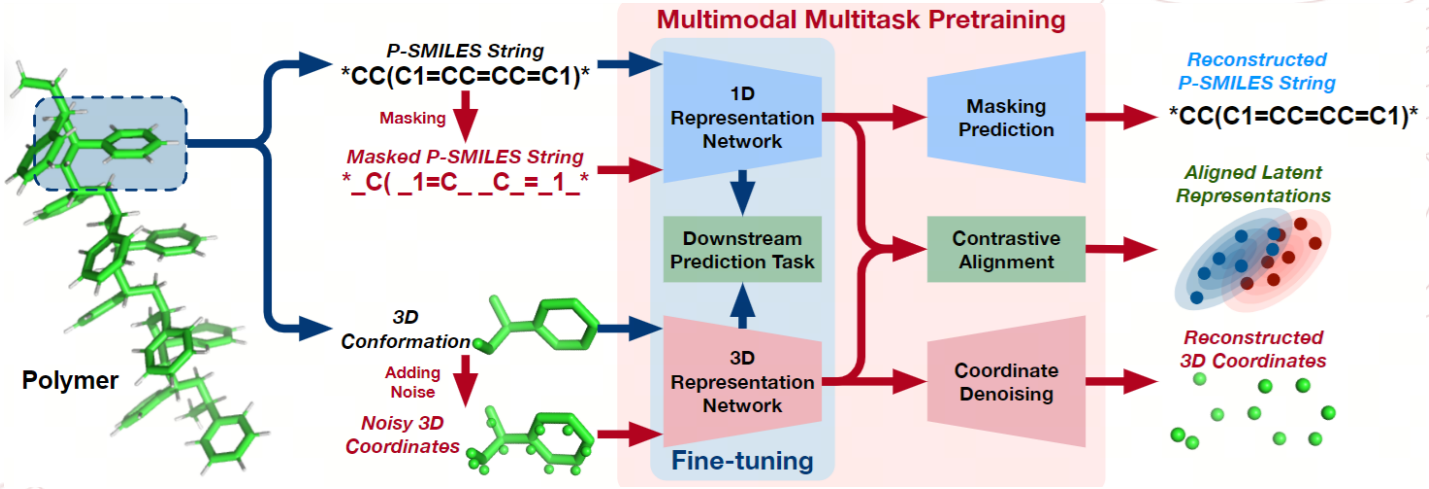
■ MMPolymer

- Typically, the properties of a polymer, such as plasticity, conductivity, bio-compatibility, and so on, are highly correlated with its **3D structure**.
- Therefore, we propose MMPolymer, a **multimodal multitask pretraining** framework incorporating polymer **1D sequential** and **3D structural** information to encourage downstream polymer property prediction tasks.



Our Approach: MMPolymer

■ Overview

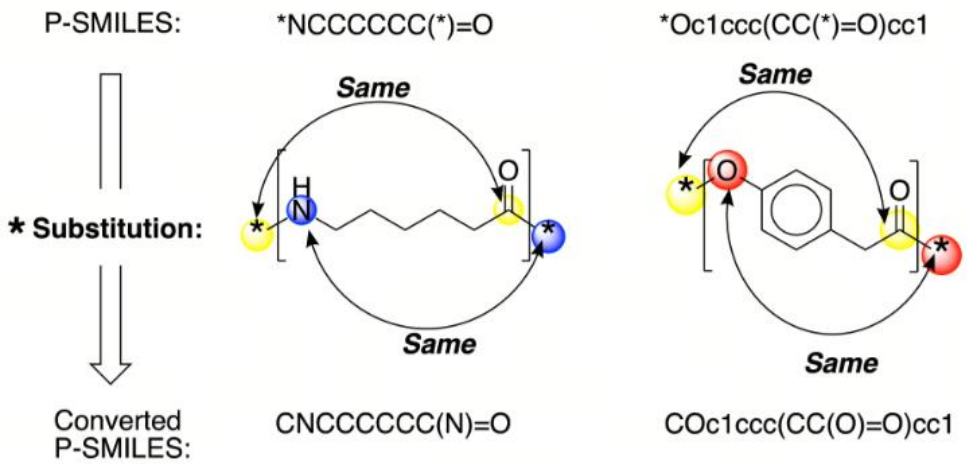


- **The first work** that incorporates 3D structural information into polymer property prediction.
- Besides, considering the scarcity of polymer 3D data, we further introduce the "**Star Substitution**" strategy to extract 3D structural information effectively.
- Experiments show that MMPolymer achieves **state-of-the-art performance** in downstream polymer property prediction tasks.

Our Approach: MMPolymer

■ Star Substitution Strategy

- Due to the scarcity of polymer 3D data, we can only leverage **the 3D conformation of the corresponding repeating unit** to approximate the whole polymer 3D conformation.
- In this case, we further introduce the "**Star Substitution**" strategy to extract 3D structural information effectively.

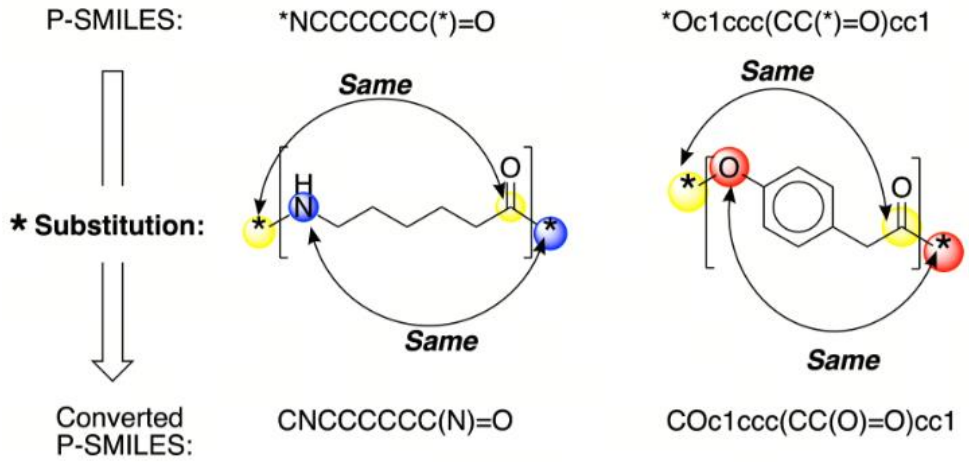


Star Substitution

The "*" symbol in the P-SMILES string is replaced by the **neighboring atom symbol** of another "*" symbol

Our Approach: MMPolymer

■ Star Substitution Strategy



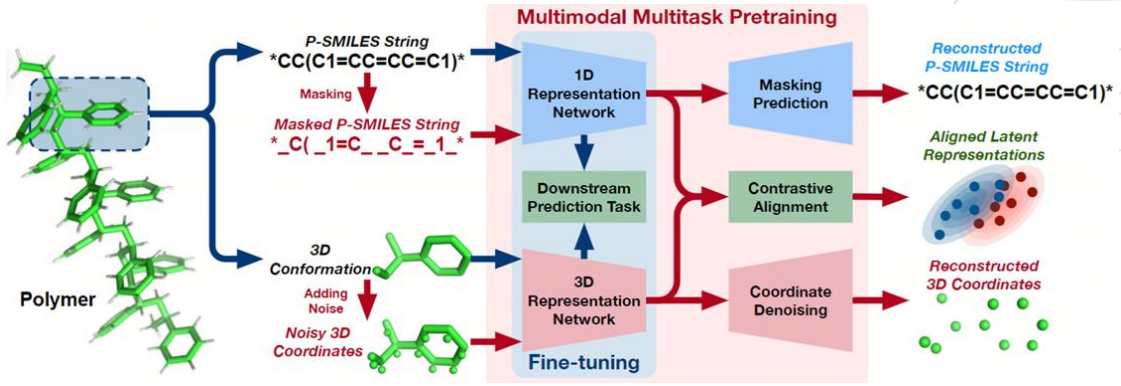
Star Substitution

The "*" symbol in the P-SMILES string is replaced by the **neighboring atom symbol** of another "*" symbol

- Then we use the RDKit tool to generate the 3D conformation based on the **converted P-SMILES string**.
- In this way, the generated 3D conformation can not only reflect 3D structural features **within repeating units** but also reflect 3D structural features **between the repeating units**, thus contributing to extracting polymer 3D structural information effectively.

Our Approach: MMPolymer

■ Multimodal Multitask Pretraining Framework



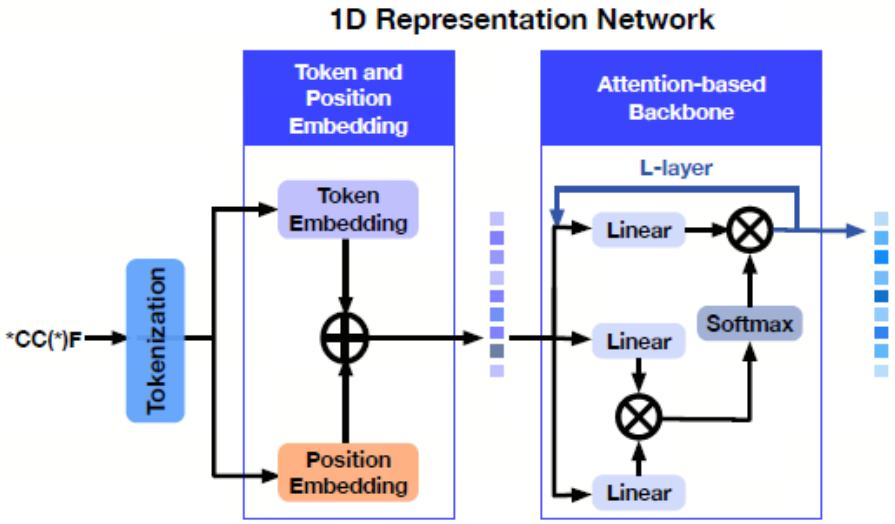
- During pretraining, we firstly **mask the P-SMILES string randomly**, **add noise to the atom coordinates of corresponding 3D conformation**, and pass them through the 1D and 3D representation networks, respectively.
- Then we learn our MMPolymer based on three pretraining tasks, including **1D Task** (predicting masked tokens), 3D Task (recovering clear 3D coordinates), and **Contrastive Learning Task** (aligning learned 1D and 3D representations):

$$\mathcal{L}_{\text{pretrain}} = \mathcal{L}_{\text{1D}} + \mathcal{L}_{\text{3D}} + \mathcal{L}_{\text{contrastive}}$$

Our Approach: MMPolymer

■ Multimodal Multitask Pretraining Framework

➢ 1D Task



$$\mathcal{L}_{1D} = -\frac{1}{|\mathcal{M}|}\sum_{i\in\mathcal{M}}\sum_{j}^{|\mathcal{V}|}\boldsymbol{y_i}[j]\cdot\log(\hat{\boldsymbol{y}}_{\boldsymbol{i}}[j])$$

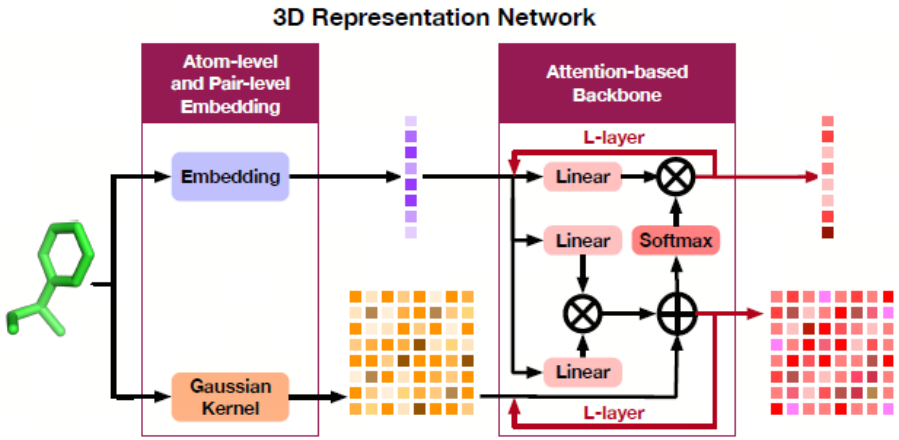
- A typical **Masked Language Modeling** task in NLP.
- Approximately 15% tokens in the polymer sequence are randomly masked. These tokens are subjected to three possiblere placement options: they may be replaced with a special token [MASK], a random token, or left unchanged.
- Then the **1D representation network** is trained to recover the **original identity** of these masked tokens based on the contextual information provided by the surrounding sequence.

Our Approach: MMPolymer

■ Multimodal Multitask Pretraining Framework

➢ 3D Task

- **Noise** is randomly introduced to atom coordinates of the given 3D conformation, thus generateing **corrupted 3D conformation** with noisy 3D atom coordinates.
- Then the **3D representation network** is trained to recover the **original 3D atom coordinates** from the corrupted 3D conformation.



$$\hat{\boldsymbol{p}}_i = \tilde{\boldsymbol{p}}_i + \sum_{j=1}^{N} \frac{\psi(\tilde{\boldsymbol{x}}_{p,ij}^{(L)} - \tilde{\boldsymbol{x}}_{p,ij}^{(0)})(\tilde{\boldsymbol{p}}_i - \tilde{\boldsymbol{p}}_j)}{N},$$

$$\mathcal{L}_{3D} = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{3}\begin{cases} 0.5|\boldsymbol{p}_i[j] - \hat{\boldsymbol{p}}_i[j]|^2, & \text{if } |\boldsymbol{p}_i[j] - \hat{\boldsymbol{p}}_i[j]| < 1, \\ |\boldsymbol{p}_i[j] - \hat{\boldsymbol{p}}_i[j]| - 0.5, & \text{otherwise.} \end{cases}$$

Our Approach: MMPolymer

■ Multimodal Multitask Pretraining Framework

➢ Contrastive Learning Task

- During pretraining, we also employ **contrastive learning** to align 1D sequential representation learned by 1D representation network and 3D structural representation learned by 3D representation network.
- In this way, 1D sequential representation and 3D structural representation of polymers are **aligned** into a shared space, thus enhancing the coherence and mutual informativeness of these multimodal representations.

$$\mathcal{L}_{\text{contrastive}} = -\frac{1}{K}\sum_{i=1}^{K}\log\left(\frac{\exp(\text{sim}(\boldsymbol{X}_{1d}^{i}, \boldsymbol{X}_{3d}^{i})/\tau)}{\sum_{j=1}^{K}\exp(\text{sim}(\boldsymbol{X}_{1d}^{i}, \boldsymbol{X}_{3d}^{j})/\tau)}\right)$$

Experiments

Experimental Setup

Datasets

Table 1: The summary of our datasets, where the pretraining dataset is unlabeled and the fine-tuning datasets are regression-type datasets with corresponding property labels.

Dataset	Property	Data Range	Data Size
PI1M	/	/	~1M
Egc	bandgap (chain)	[0.02, 8.30]	3380
Egb	bandgap (bulk)	[0.39, 10.05]	561
Eea	electron affinity	[0.39, 4.61]	368
Ei	ionization energy	[3.55, 9.61]	370
Xc	crystallization tendency	[0.13, 98.41]	432
EPS	dielectric constant	[2.61, 8.52]	382
Nc	refractive index	[1.48, 2.58]	382
Eat	atomization energy	[−6.83, −5.02]	390

- We use the **PI1M** dataset, which contains about one million unlabeled polymer data, to pretrain our MMPolymer.
- The widely used open-source polymer property datasets (denoted as **Egc**, **Egb**, **Eea**, **Ei**, **Xc**, **EPS**, **Nc**, and **Eat**, respectively) are used as our fine-tuning datasets.

Experiments

■ Experimental Setup

➢ Baselines

- **Polymer pretraining methods:**

  Including SML, PLM, polyBERT and Transpolymer

- **Molecular pretraining methods:**

  Including ChemBERTa, MolCLR, 3D Infomax and Uni-Mol

➢ Evaluation Metrics

- Since property prediction tasks on the fine-tuning datasets are all regression tasks, we also choose **root mean squared error (RMSE)** and **R-squared (R^2)** as evaluation metrics in line with previous works, thus guaranteeing a comprehensive and fair assessment of the predictive performance.

Experiments

Performance

Table 2: The performance comparison of different methods on eight polymer property datasets, and the best result for each polymer property dataset has been bolded.

Metric	Method	Egc	Egb	Eea	Ei	Xc	EPS	Nc	Eat
RMSE (↓)	ChemBERTa [1]	$0.539_{\pm 0.049}$	$0.664_{\pm 0.079}$	$0.350_{\pm 0.036}$	$0.485_{\pm 0.086}$	$18.711_{\pm 1.396}$	$0.603_{\pm 0.083}$	$0.140_{\pm 0.010}$	$0.219_{\pm 0.056}$
	MolCLR [49]	$0.587_{\pm 0.024}$	$0.644_{\pm 0.072}$	$0.404_{\pm 0.017}$	$0.533_{\pm 0.053}$	$21.719_{\pm 1.631}$	$0.631_{\pm 0.045}$	$0.117_{\pm 0.015}$	$0.094_{\pm 0.033}$
	3D Infomax [40]	$0.494_{\pm 0.039}$	$0.553_{\pm 0.032}$	$0.335_{\pm 0.055}$	$0.449_{\pm 0.086}$	$19.483_{\pm 2.491}$	$0.582_{\pm 0.054}$	$0.101_{\pm 0.018}$	$0.094_{\pm 0.039}$
	Uni-Mol [58]	$0.489_{\pm 0.028}$	$0.531_{\pm 0.055}$	$0.332_{\pm 0.027}$	$0.407_{\pm 0.080}$	$17.414_{\pm 1.581}$	$0.536_{\pm 0.053}$	$0.095_{\pm 0.013}$	$0.084_{\pm 0.034}$
	SML [55]	$0.489_{\pm 0.056}$	$0.547_{\pm 0.110}$	$0.313_{\pm 0.016}$	$0.432_{\pm 0.060}$	$18.981_{\pm 1.258}$	$0.576_{\pm 0.020}$	$0.102_{\pm 0.010}$	$0.062_{\pm 0.014}$
	PLM [55]	$0.459_{\pm 0.036}$	$0.528_{\pm 0.081}$	$0.322_{\pm 0.037}$	$0.444_{\pm 0.062}$	$19.181_{\pm 1.308}$	$0.576_{\pm 0.060}$	$0.100_{\pm 0.010}$	$\mathbf{0.050}_{\pm 0.010}$
	polyBERT [19]	$0.553_{\pm 0.011}$	$0.759_{\pm 0.042}$	$0.363_{\pm 0.037}$	$0.526_{\pm 0.068}$	$18.437_{\pm 0.560}$	$0.618_{\pm 0.049}$	$0.113_{\pm 0.003}$	$0.172_{\pm 0.016}$
	Transpolymer [52]	$0.453_{\pm 0.007}$	$0.576_{\pm 0.021}$	$0.326_{\pm 0.040}$	$0.397_{\pm 0.061}$	$17.740_{\pm 0.732}$	$0.547_{\pm 0.051}$	$0.096_{\pm 0.016}$	$0.147_{\pm 0.093}$
	MMPolymer (ours)	$\mathbf{0.431}_{\pm 0.017}$	$\mathbf{0.496}_{\pm 0.031}$	$\mathbf{0.286}_{\pm 0.029}$	$\mathbf{0.390}_{\pm 0.057}$	$\mathbf{16.814}_{\pm 0.867}$	$\mathbf{0.511}_{\pm 0.035}$	$\mathbf{0.087}_{\pm 0.010}$	$0.061_{\pm 0.016}$
R^2 (↑)	ChemBERTa [1]	$0.880_{\pm 0.023}$	$0.881_{\pm 0.028}$	$0.888_{\pm 0.035}$	$0.745_{\pm 0.102}$	$0.365_{\pm 0.098}$	$0.682_{\pm 0.123}$	$0.643_{\pm 0.076}$	$0.590_{\pm 0.078}$
	MolCLR [49]	$0.858_{\pm 0.010}$	$0.882_{\pm 0.027}$	$0.854_{\pm 0.038}$	$0.689_{\pm 0.037}$	$0.176_{\pm 0.026}$	$0.683_{\pm 0.020}$	$0.764_{\pm 0.037}$	$0.885_{\pm 0.104}$
	3D Infomax [40]	$0.900_{\pm 0.016}$	$0.898_{\pm 0.018}$	$0.891_{\pm 0.045}$	$0.766_{\pm 0.086}$	$0.274_{\pm 0.122}$	$0.690_{\pm 0.063}$	$0.797_{\pm 0.086}$	$0.869_{\pm 0.097}$
	Uni-Mol [58]	$0.901_{\pm 0.013}$	$0.925_{\pm 0.011}$	$0.901_{\pm 0.027}$	$0.820_{\pm 0.075}$	$0.454_{\pm 0.079}$	$0.751_{\pm 0.085}$	$0.828_{\pm 0.072}$	$0.937_{\pm 0.032}$
	SML [55]	$0.901_{\pm 0.022}$	$0.920_{\pm 0.029}$	$0.915_{\pm 0.015}$	$0.802_{\pm 0.051}$	$0.340_{\pm 0.125}$	$0.726_{\pm 0.038}$	$0.812_{\pm 0.058}$	$0.967_{\pm 0.015}$
	PLM [55]	$0.911_{\pm 0.014}$	$0.925_{\pm 0.021}$	$0.910_{\pm 0.019}$	$0.791_{\pm 0.049}$	$0.330_{\pm 0.105}$	$0.726_{\pm 0.058}$	$0.817_{\pm 0.056}$	$\mathbf{0.980}_{\pm 0.008}$
	polyBERT [19]	$0.875_{\pm 0.006}$	$0.844_{\pm 0.034}$	$0.880_{\pm 0.035}$	$0.705_{\pm 0.085}$	$0.384_{\pm 0.066}$	$0.681_{\pm 0.058}$	$0.769_{\pm 0.034}$	$0.672_{\pm 0.119}$
	Transpolymer [52]	$0.916_{\pm 0.002}$	$0.911_{\pm 0.008}$	$0.902_{\pm 0.036}$	$0.830_{\pm 0.059}$	$0.430_{\pm 0.058}$	$0.744_{\pm 0.075}$	$0.826_{\pm 0.071}$	$0.800_{\pm 0.172}$
	MMPolymer (ours)	$\mathbf{0.924}_{\pm 0.006}$	$\mathbf{0.934}_{\pm 0.008}$	$\mathbf{0.925}_{\pm 0.025}$	$\mathbf{0.836}_{\pm 0.053}$	$\mathbf{0.488}_{\pm 0.072}$	$\mathbf{0.779}_{\pm 0.052}$	$\mathbf{0.864}_{\pm 0.036}$	$0.961_{\pm 0.018}$

State-of-the-art performance !

Experiments

Performance

- We also explore the predictive capacity of our MMPolymer when **only utilizing single modality information** (either polymer 1D sequential information or 3D structural information) during fine-tuning.

Table 3: The performance improvement of MMPolymer-1D, which only utilizes polymer 1D sequential information during fine-tuning, and MMPolymer-3D, which only utilizes 3D structural information during fine-tuning, compared with the best baseline on each polymer property dataset.

Dataset	MMPolymer-1D		MMPolymer-3D	
	ΔRMSE (↓)	ΔR^2 (↑)	ΔRMSE (↓)	ΔR^2 (↑)
Egc	**-0.008**	**+0.003**	**-0.004**	**+0.001**
Egb	**-0.015**	**+0.005**	**-0.025**	**+0.007**
Eea	**-0.009**	**+0.002**	**-0.027**	**+0.010**
Ei	+0.016	-0.011	**-0.003**	**+0.004**
Xc	**-0.219**	**+0.010**	+0.449	-0.028
EPS	**-0.011**	**+0.016**	**-0.025**	**+0.028**
Nc	**-0.005**	**+0.024**	**-0.006**	**+0.025**
Eat	+0.028	-0.046	+0.011	-0.019

Great adaptability !

Experiments

➢ Ablation Studies

Table 4: The performance of MMPolymer under different data processing strategies, where the "Star Keep" strategy refers to directly using the original P-SMILES string, the "Star Remove" strategy refers to removing "*" symbols in the original P-SMILES string and the "Star Substitution" strategy refers to replacing the "*" symbol in the original P-SMILES string with the neighboring atom symbol of another "*" symbol.

Metric	Strategy	Egc	Egb	Eea	Ei	Xc	EPS	Nc	Eat
RMSE (↓)	Star Keep	$0.433_{\pm 0.015}$	$0.506_{\pm 0.055}$	$0.310_{\pm 0.022}$	$0.392_{\pm 0.047}$	$16.836_{\pm 1.272}$	$0.514_{\pm 0.047}$	$0.089_{\pm 0.011}$	$0.077_{\pm 0.042}$
	Star Remove	$0.478_{\pm 0.023}$	$0.527_{\pm 0.012}$	$0.299_{\pm 0.016}$	$0.403_{\pm 0.041}$	$16.962_{\pm 0.803}$	$0.514_{\pm 0.032}$	$0.091_{\pm 0.011}$	$0.083_{\pm 0.040}$
	Star Substitution (Ours)	$\mathbf{0.431}_{\pm 0.017}$	$\mathbf{0.496}_{\pm 0.031}$	$\mathbf{0.286}_{\pm 0.029}$	$\mathbf{0.390}_{\pm 0.057}$	$\mathbf{16.814}_{\pm 0.867}$	$\mathbf{0.511}_{\pm 0.035}$	$\mathbf{0.087}_{\pm 0.010}$	$\mathbf{0.061}_{\pm 0.016}$
R^2 (↑)	Star Keep	$0.921_{\pm 0.006}$	$0.927_{\pm 0.008}$	$0.914_{\pm 0.022}$	$0.833_{\pm 0.049}$	$0.483_{\pm 0.102}$	$0.778_{\pm 0.055}$	$0.855_{\pm 0.038}$	$0.945_{\pm 0.041}$
	Star Remove	$0.905_{\pm 0.009}$	$0.925_{\pm 0.013}$	$0.921_{\pm 0.015}$	$0.828_{\pm 0.043}$	$0.471_{\pm 0.093}$	$0.776_{\pm 0.050}$	$0.845_{\pm 0.053}$	$0.938_{\pm 0.040}$
	Star Substitution (Ours)	$\mathbf{0.924}_{\pm 0.006}$	$\mathbf{0.934}_{\pm 0.008}$	$\mathbf{0.925}_{\pm 0.025}$	$\mathbf{0.836}_{\pm 0.053}$	$\mathbf{0.488}_{\pm 0.072}$	$\mathbf{0.779}_{\pm 0.052}$	$\mathbf{0.864}_{\pm 0.036}$	$\mathbf{0.961}_{\pm 0.018}$

The effectiveness of our "Star Substitution" strategy

Experiments

➢ Ablation Studies

Table 5: The performance of MMPolymer under different pretraining settings, where "1D pre" refers to the masking predictio task on the 1D representation network, "3D pre" refers to the coordinate denoising task on the 3D representation network, an "Contrast" refers to the cross-modal alignment task.

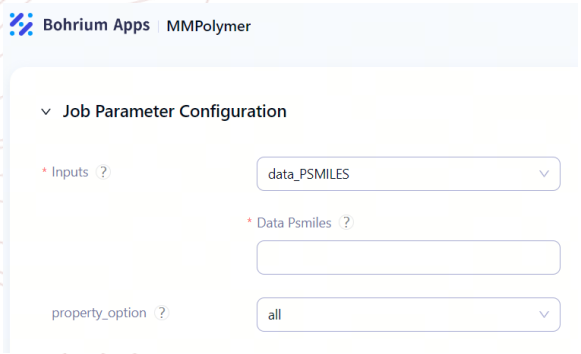
Metric	1D pre	3D pre	Contrast	Egc	Egb	Eea	Ei	Xc	EPS	Nc	Eat
RMSE (↓)	×	×	×	$0.596_{\pm 0.022}$	$0.575_{\pm 0.031}$	$0.343_{\pm 0.029}$	$0.432_{\pm 0.062}$	$20.152_{\pm 1.624}$	$0.569_{\pm 0.053}$	$0.102_{\pm 0.010}$	$0.122_{\pm 0.051}$
	✓	×	×	$0.438_{\pm 0.010}$	$0.510_{\pm 0.034}$	$0.311_{\pm 0.028}$	$0.394_{\pm 0.058}$	$16.818_{\pm 0.779}$	$0.535_{\pm 0.052}$	$0.091_{\pm 0.008}$	$0.112_{\pm 0.085}$
	×	✓	×	$0.492_{\pm 0.026}$	$0.542_{\pm 0.042}$	$0.337_{\pm 0.023}$	$0.424_{\pm 0.080}$	$18.542_{\pm 0.849}$	$0.532_{\pm 0.049}$	$0.096_{\pm 0.015}$	$0.086_{\pm 0.030}$
	×	×	✓	$0.618_{\pm 0.013}$	$0.716_{\pm 0.058}$	$0.392_{\pm 0.041}$	$0.456_{\pm 0.079}$	$19.624_{\pm 2.003}$	$0.632_{\pm 0.031}$	$0.119_{\pm 0.015}$	$0.162_{\pm 0.094}$
	✓	×	✓	$0.459_{\pm 0.010}$	$0.519_{\pm 0.044}$	$0.298_{\pm 0.032}$	$0.417_{\pm 0.048}$	$17.033_{\pm 0.482}$	$0.545_{\pm 0.062}$	$0.092_{\pm 0.012}$	$0.124_{\pm 0.073}$
	×	✓	✓	$0.593_{\pm 0.018}$	$0.574_{\pm 0.037}$	$0.347_{\pm 0.032}$	$0.421_{\pm 0.053}$	$17.816_{\pm 1.417}$	$0.560_{\pm 0.075}$	$0.104_{\pm 0.011}$	$0.140_{\pm 0.056}$
	✓	✓	×	$0.440_{\pm 0.017}$	$0.502_{\pm 0.051}$	$0.308_{\pm 0.030}$	$0.400_{\pm 0.062}$	$17.177_{\pm 0.554}$	$0.532_{\pm 0.055}$	$0.092_{\pm 0.011}$	$0.115_{\pm 0.084}$
	✓	✓	✓	$\mathbf{0.431}_{\pm 0.017}$	$\mathbf{0.496}_{\pm 0.031}$	$\mathbf{0.286}_{\pm 0.029}$	$\mathbf{0.390}_{\pm 0.057}$	$\mathbf{16.814}_{\pm 0.867}$	$\mathbf{0.511}_{\pm 0.035}$	$\mathbf{0.087}_{\pm 0.010}$	$\mathbf{0.061}_{\pm 0.016}$
R^2 (↑)	×	×	×	$0.854_{\pm 0.010}$	$0.910_{\pm 0.019}$	$0.895_{\pm 0.025}$	$0.799_{\pm 0.064}$	$0.269_{\pm 0.090}$	$0.725_{\pm 0.079}$	$0.811_{\pm 0.040}$	$0.873_{\pm 0.082}$
	✓	×	×	$0.921_{\pm 0.005}$	$0.931_{\pm 0.003}$	$0.914_{\pm 0.020}$	$0.833_{\pm 0.054}$	$\mathbf{0.488}_{\pm 0.061}$	$0.757_{\pm 0.065}$	$0.847_{\pm 0.050}$	$0.878_{\pm 0.137}$
	×	✓	×	$0.900_{\pm 0.012}$	$0.921_{\pm 0.013}$	$0.897_{\pm 0.029}$	$0.803_{\pm 0.079}$	$0.378_{\pm 0.077}$	$0.758_{\pm 0.069}$	$0.824_{\pm 0.080}$	$0.937_{\pm 0.026}$
	×	×	✓	$0.843_{\pm 0.002}$	$0.862_{\pm 0.022}$	$0.862_{\pm 0.037}$	$0.773_{\pm 0.090}$	$0.303_{\pm 0.125}$	$0.665_{\pm 0.060}$	$0.744_{\pm 0.058}$	$0.753_{\pm 0.158}$
	✓	×	✓	$0.913_{\pm 0.004}$	$0.928_{\pm 0.006}$	$0.919_{\pm 0.024}$	$0.816_{\pm 0.047}$	$0.474_{\pm 0.067}$	$0.741_{\pm 0.094}$	$0.837_{\pm 0.066}$	$0.865_{\pm 0.107}$
	×	✓	✓	$0.855_{\pm 0.007}$	$0.910_{\pm 0.021}$	$0.892_{\pm 0.026}$	$0.810_{\pm 0.056}$	$0.422_{\pm 0.105}$	$0.730_{\pm 0.093}$	$0.803_{\pm 0.042}$	$0.827_{\pm 0.087}$
	✓	✓	×	$0.921_{\pm 0.005}$	$0.933_{\pm 0.009}$	$0.915_{\pm 0.020}$	$0.827_{\pm 0.060}$	$0.466_{\pm 0.060}$	$0.758_{\pm 0.072}$	$0.847_{\pm 0.034}$	$0.871_{\pm 0.135}$
	✓	✓	✓	$\mathbf{0.924}_{\pm 0.006}$	$\mathbf{0.934}_{\pm 0.008}$	$\mathbf{0.925}_{\pm 0.025}$	$\mathbf{0.836}_{\pm 0.053}$	$\mathbf{0.488}_{\pm 0.072}$	$\mathbf{0.779}_{\pm 0.052}$	$\mathbf{0.864}_{\pm 0.036}$	$\mathbf{0.961}_{\pm 0.018}$

The effectiveness of our multimodal multitask pretraining paradigm

Conclusion

- In this work, we present MMPolymer, a **multimodal multitask pretraining** framework, to predict polymer properties.
- Through effectively combining polymer **1D sequential** and **3D structural** information, MMPolymer can fully capture diverse aspects of polymer data, creating **a promising model** for downstream polymer property prediction tasks.
- The extensive experiments consistently demonstrate that MMPolymer achieves **state-of-the-art performance** on various polymer property prediction tasks, significantly outperforming existing polymer property prediction methods.

Bohrium APP



Online Platform

https://bohrium.dp.tech/apps/mmpolymer

Thank You & QA

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