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Paper Code

Graph Positional Autoencoders as Self-supervised Learners

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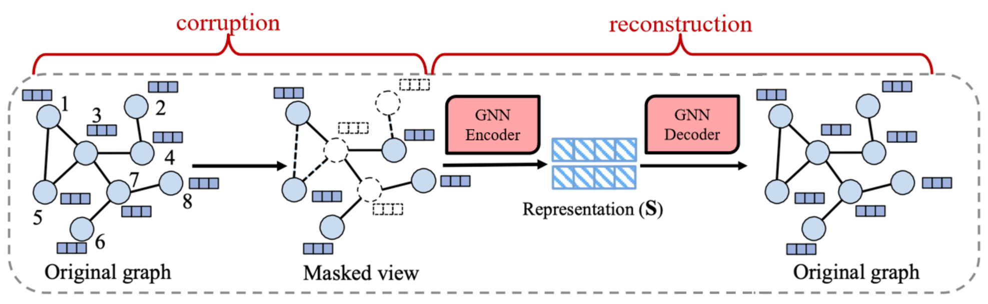
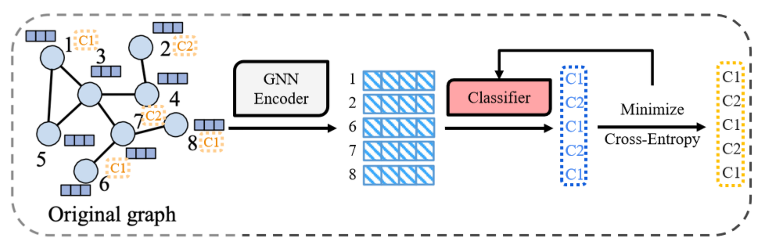
❖ Motivation

➢ Background

Masked Graph Autoencoders (GAEs) follow a corruption-reconstruction framework, which learns graph representations by recovering the missing information of the incomplete input graphs.



Pre-training of Masked Graph Autoencoders



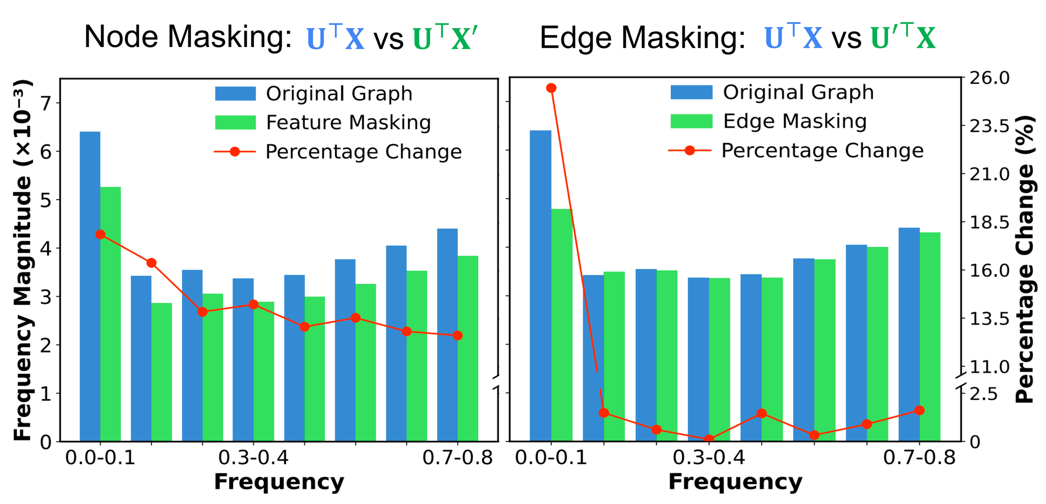
Fine-tuning for downstream task

➢ Limitations of existing methods

Existing masked GAEs tend to focus on reconstructing low-frequency information of graphs while overlooking high-frequency information.

Model	Corruption			Reconstruction		
	Feature	Edge	Position	Feature	Edge	Other
GraphMAE [18]	✓	-	-	✓	-	-
StructMAE [32]	✓	-	-	✓	-	-
AUG-MAE [59]	✓	-	-	✓	-	-
S2GAE [50]	-	✓	-	-	✓	-
SeeGera [30]	✓	✓	-	✓	✓	-
Bandana [77]	-	✓	-	-	✓	-
MaskGAE [28]	-	✓	-	✓	-	Degree
GiGaMAE [45]	✓	✓	-	-	-	Latent
GraphPAE	✓	-	✓	✓	-	Position

Comparison between different masked graph autoencoders.



Comparison of the frequency magnitudes between original and corrupted graphs.

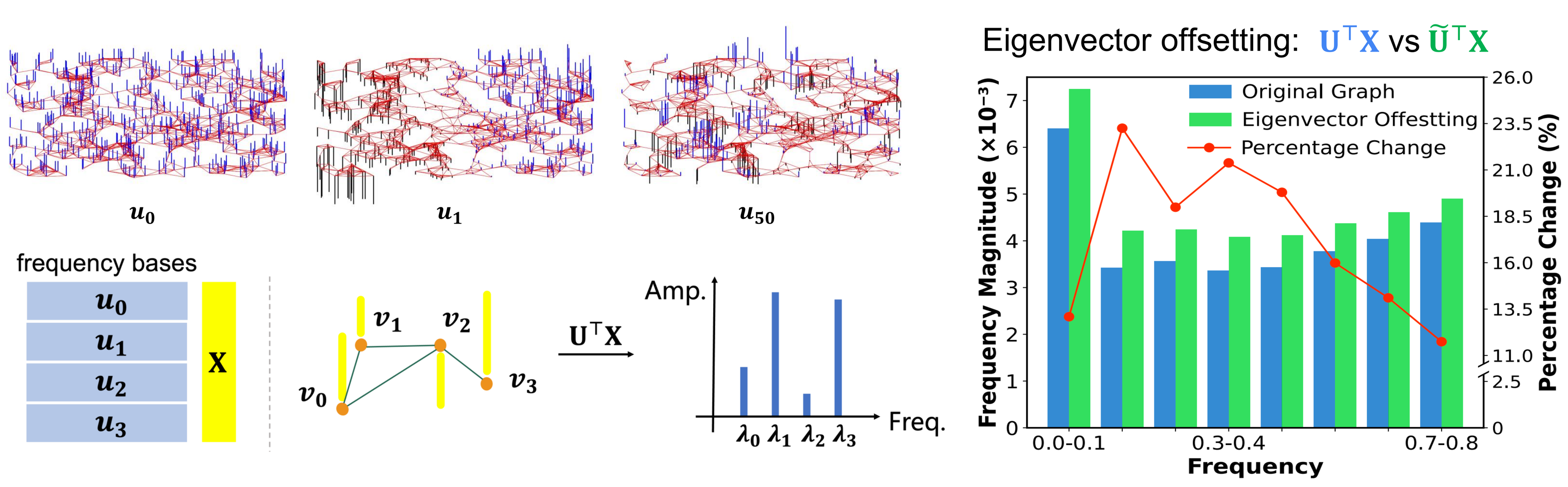
➢ Our Goal

To equip GAEs with the ability to exploit the diverse frequency information.

❖ Inspired by Spectral Theory

➢ A Spectral Perspective on the Corruption Strategy

Eigenvectors of the graph Laplacian represent different frequencies, acting as frequency bases in the spectral domain.

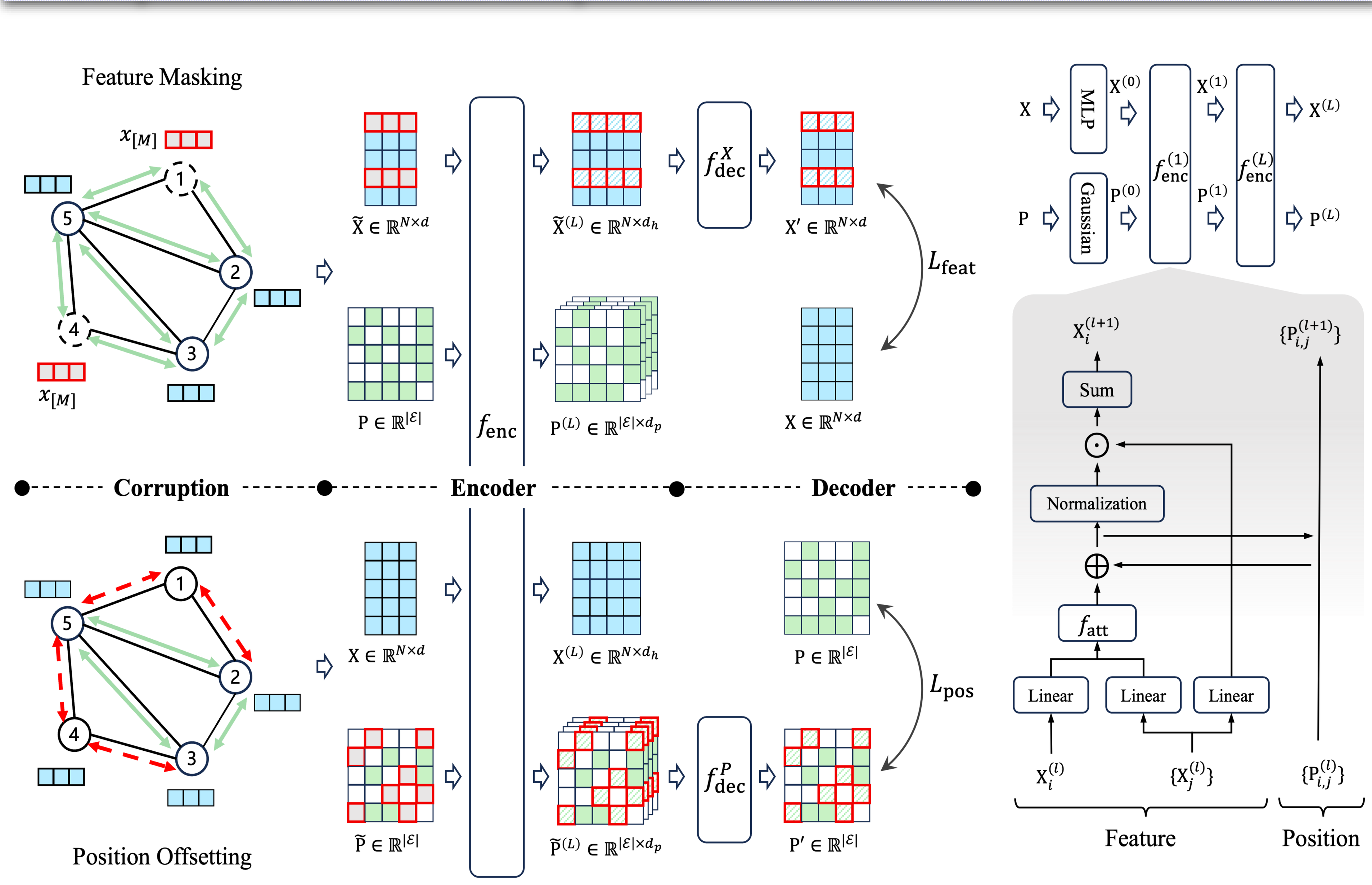


➢ Eigenvectors as Positional Encoding

Eigenvectors are utilized as enhanced features (positional encodings) to boost expressivity of MPNN.

Incorporating eigenvector, *i.e.*, position, corruption-reconstruction into masked GAEs.

❖ Proposed Framework: GraphPAE



- ➢ **GraphPAE** uses a dual-path architecture to separately reconstruct node features and positions, overcoming the expressivity and ambiguity challenges.
- **Feature Path:** Integrates positional encodings to enhance message-passing expressivity for improved feature reconstruction.
- **Position Path:** Leverages node representations to refine positional encodings, enabling the model to learn diverse frequency information.
- **Reconstruction Strategy:** Reconstructs relative node distances as a surrogate objective to avoid the ambiguity of eigenvectors.

➢ Encoder

$$\mathbf{X}_i^{(l+1)}, \mathbf{P}_i^{(l+1)} = f_{\text{enc}}^{(l+1)}\left(\mathbf{X}_i^{(l)}, \left\{\mathbf{X}_j^{(l)}\right\}_{j\in\mathcal{N}_i}, \mathbf{P}_i^{(l)}\right)$$

$$\alpha_{i,j}^{(l)} = f_{\text{att}}\left(\mathbf{X}_i^{(l)}, \mathbf{X}_j^{(l)}\right), \quad \alpha_{i,j}^{(l)} \in \mathbb{R}^d,$$

$$\mathbf{X}_i^{(l+1)} = \sum_{j\in\mathcal{N}_i}\left(\alpha_{i,j}^{(l)} + \mathbf{P}_{i,j}^{(l)}\right) \odot \text{MLP}\left(\mathbf{X}_j^{(l)}\right)$$

$$\mathbf{P}_{i,j}^{(l+1)} = \alpha_{i,j}^{(l)} + \mathbf{P}_{i,j}^{(l)}.$$

➢ Decoder

$$\mathcal{L}_{\text{feat}} = \frac{1}{|\widetilde{\mathcal{V}}|}\sum_{v_i\in\widetilde{\mathcal{V}}}\left(1 - \frac{\mathbf{X}_i^T\mathbf{X}_i'}{\|\mathbf{X}_i\|\cdot\|\mathbf{X}_i'\|}\right)^\gamma$$

$$\mathcal{L}_{\text{pos}}^{i,j} = \begin{cases} \frac{\left(\mathbf{P}'_{i,j}-\mathbf{P}_{i,j}\right)^2}{2}, & \text{if } |\mathbf{P}'_{i,j} - \mathbf{P}_{i,j}| < 1 \\ |\mathbf{P}'_{i,j} - \mathbf{P}_{i,j}| - \frac{1}{2}, & \text{otherwise} \end{cases}$$

$$\mathcal{L}_{\text{pos}} = \frac{1}{\sum_{v_i\in\widetilde{\mathcal{V}}}|\mathcal{N}_i|}\sum_{v_i\in\widetilde{\mathcal{V}}, j\in\mathcal{N}_i}\mathcal{L}_{\text{pos}}^{i,j}$$

❖ Experiments

➢ Performance of Node Classification

Dataset	Small Graphs				Large Graphs	
	BlogCatalog	Chameleon	Squirrel	Actor	arXiv-year	Penn94
Supervised	80.52±2.10	80.02±0.87	71.91±1.03	33.93±2.47	46.02±0.26	81.53±0.55
DGI	72.07±0.16	43.83±0.14	34.56±0.10	27.98±0.09	-	-
BGRL	79.74±0.46	61.24±1.07	43.24±0.52	26.61±0.57	41.43±0.04	63.31±0.49
MVGRL	63.24±0.94	73.19±0.42	60.09±0.44	34.64±0.20	-	-
CCA-SSG	74.00±0.28	75.00±0.75	61.58±1.98	27.79±0.58	40.78±0.01	62.63±0.20
Sp^2GCL	72.73±0.46	78.88±1.04	62.61±0.87	34.70±0.92	39.09±0.02	68.80±0.45
VGAE	60.47±1.84	62.32±1.90	42.50±1.35	31.57±0.75	36.39±0.21	55.31±0.28
GraphMAE	79.90±1.13	79.50±0.57	61.13±0.60	32.15±1.33	40.30±0.04	67.97±0.21
GraphMAE2	77.34±0.12	79.13±0.19	70.27±0.88	34.48±0.26	38.97±0.03	67.86±0.42
MaskGAE	73.10±0.08	74.50±0.87	68.53±0.44	33.44±0.34	40.59±0.04	63.84±0.03
S2GAE	75.76±0.43	60.24±0.37	68.60±0.56	26.17±0.38	40.32±0.12	70.24±0.09
AUG-MAE	82.03±0.69	70.10±1.88	62.57±0.67	33.42±0.38	37.10±0.13	69.90±0.43
GraphPAE	**85.76±1.22**	**80.51±1.25**	**72.05±1.40**	**38.55±1.35**	**41.85±0.04**	**71.79±0.37**

➢ Performance of Graph Prediction

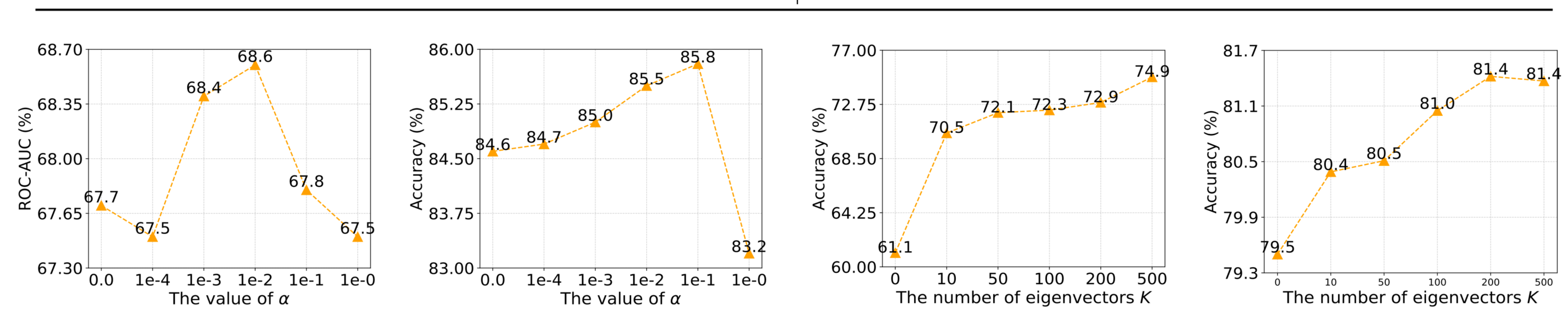
Task	Regression (Metric: RMSE ↓)			Classification (Metric: ROC-AUC% ↑)			
Dataset	molesol	molipo	molfreesolv	molbace	molbbbp	molclintox	moltocx21
Supervised	1.173±0.057	0.757±0.018	2.755±0.349	80.42±0.96	68.17±1.48	88.14±2.51	74.91±0.51
InfoGraph	1.344±0.178	1.005±0.023	10.005±8.147	73.64±3.64	66.33±2.79	64.50±5.32	69.74±0.57
GraphCL	1.272±0.089	0.910±0.016	7.679±2.748	73.32±2.70	68.22±2.19	74.92±4.42	72.40±1.07
MVGRL	1.433±0.145	0.962±0.036	9.024±1.982	74.88±1.43	67.24±3.19	73.84±2.75	70.48±0.83
JOAO	1.285±0.121	0.865±0.032	5.131±0.782	74.43±1.94	67.62±1.29	71.28±4.12	71.38±0.92
Sp^2GCL	1.235±0.119	0.835±0.026	4.144±0.573	78.76±1.43	**68.72±1.53**	80.88±3.86	73.06±0.75
GraphMAE	1.050±0.034	0.850±0.022	2.740±0.233	79.14±1.31	66.55±1.78	80.56±5.55	73.84±0.58
GraphMAE2	1.225±0.081	0.885±0.019	2.913±0.293	80.74±1.53	67.67±1.44	75.75±3.65	72.93±0.69
StructMAE	1.499±0.043	1.089±0.002	2.568±0.262	77.75±0.42	65.66±1.16	79.42±4.56	71.13±0.61
AUG-MAE	1.248±0.026	0.917±0.013	2.395±0.158	78.54±2.49	67.05±0.63	82.66±1.98	74.33±0.07
GraphPAE	**1.015±0.045**	**0.810±0.018**	**2.058±0.188**	**81.11±1.24**	68.56±0.71	**82.69±3.39**	**74.46±0.54**

➢ Performance of Transfer Learning on QM9

Target	μ	α	ϵ_{homo}	ϵ_{lumo}	Δ_ϵ	R^2	ZPVE	U_0	U	H	G	C_v
Unit	D	a_0^3	10^{-2}meV	10^{-2}meV	10^{-2}meV	a_0^2	10^{-2}meV	meV	meV	meV	meV	cal/mol/K
GraphCL	1.035	2.321	2.030	3.667	4.523	40.725	2.063	2.461	1.745	1.734	1.751	1.747
GraphMAE	1.030	2.924	2.407	6.373	4.813	41.955	4.623	1.411	2.207	2.208	2.207	2.200
Mole-BERT	1.031	1.918	1.477	4.127	4.240	44.374	2.190	2.532	2.509	2.511	2.516	2.508
SimSGT	1.064	2.413	2.837	4.227	4.107	40.504	2.127	1.948	2.420	2.416	2.416	2.410
GraphPAE	**0.703**	**0.879**	**1.199**	**2.141**	**2.289**	**36.480**	**0.502**	**0.510**	**0.639**	**0.639**	**0.641**	**0.643**

➢ Ablation Studies

Exp	Corrupt Info.		Recon Info.		Dual-Path	Node-level		Graph-level		
No.	Feature	Position	Feature	Position		Blog (↑)	Squirrel (↑)	Bace (↑)	Bbbp (↑)	Freesolv (↓)
a	✓	✓	✓			82.8±1.7	66.4±1.6	78.4±1.2	66.4±1.7	2.79±0.40
b	✓	✓	✓	✓		83.5±1.0	68.5±0.9	78.9±2.1	66.8±0.6	2.44±0.36
c	✓		✓			84.6±1.6	71.3±0.9	79.4±3.4	67.7±0.9	2.20±0.14
d	✓	✓	✓	✓	✓	**85.8±1.2**	**72.1±1.4**	**81.1±1.2**	**68.6±0.7**	**2.06±0.19**



(a) Molbbbp (b) BlogCatalog (c) Squirrel (d) Chameleon