

Table 1: Ablation on Zinc-12k dataset (MAE \downarrow). Highlighted are the **first**, **second** results.

MODEL	NODE PE/SE	EDGERWSE	HODGE1LAP	TEST MAE
GINE	RWSE	FULL-EDGERWSE	-	0.069 ± 0.003
GINE	INTER-RWSE	INTER-RWSE	-	0.083 ± 0.006
GINE	RWSE	CELLULAR	-	0.068 ± 0.003
GAT	-	-	-	0.384 ± 0.007
GAT	-	UNDIRECTED	-	0.163 ± 0.008
GAT	-	-	PROJECT	0.130 ± 0.005
PNA	-	-	-	0.188 ± 0.004
PNA	-	UNDIRECTED	-	0.104 ± 0.004
PNA	-	-	PROJECT	0.074 ± 0.005
SSWL+	-	-	-	0.070 ± 0.005
SSWL+	-	UNDIRECTED	-	0.067 ± 0.005
SSWL+	-	-	PROJECT	0.066 ± 0.003
GPS	-	-	-	0.113 ± 0.005
GPS	RWSE	-	-	0.070 ± 0.004
GPS	RWSE	UNDIRECTED	-	0.068 ± 0.004
GPS	RWSE	-	PROJECT	0.064 ± 0.003
GRIT	-	-	-	0.149 ± 0.008
GRIT	RWSE	-	-	0.081 ± 0.010
GRIT	SPDPE	-	-	0.067 ± 0.002
GRIT	RDPE	-	-	0.059 ± 0.003
GRIT	RRWP	-	-	0.059 ± 0.002
GRIT	-	UNDIRECTED	-	0.103 ± 0.006
GRIT	-	-	PROJECT	0.086 ± 0.005
GRIT	RRWP	UNDIRECTED	-	0.058 ± 0.002
GRIT	RRWP	-	PROJECT	0.057 ± 0.003

Table 2: Experiments on three datasets from long-range graph benchmarks (LRGB). Highlighted are the **first**, **second** test results.

MODEL	PEPTIDES-FUNC (AP \uparrow)	PEPTIDES-STRUCT (MAE \downarrow)	PCQM-CONTACT (MRR \uparrow)
GCN	0.5930 ± 0.0023	0.3496 ± 0.0013	0.3234 ± 0.0006
GINE	0.5498 ± 0.0079	0.3547 ± 0.0045	0.3180 ± 0.0027
GATEDGCN	0.5864 ± 0.0077	0.3420 ± 0.0013	0.3218 ± 0.0011
TRANSFORMER+LAPPE	0.6326 ± 0.0126	0.2529 ± 0.0016	0.3174 ± 0.0020
SAN (?)+LAPPE	0.6384 ± 0.0121	0.2683 ± 0.0043	0.3350 ± 0.0003
SAN+RWSE	0.6439 ± 0.0075	0.2545 ± 0.0012	0.3350 ± 0.0003
GPS	0.6535 ± 0.0041	0.2500 ± 0.0005	0.3337 ± 0.0006
GATEDGCN+EDGERWSE	0.6002 ± 0.0048	0.2679 ± 0.0015	0.3342 ± 0.0008
GATEDGCN+HODGE1LAP	0.5926 ± 0.0059	0.2632 ± 0.0008	0.3336 ± 0.0004
GPS+EDGERWSE	0.6625 ± 0.0042	0.2501 ± 0.0012	0.3408 ± 0.0003
GPS+HODGE1LAP	0.6584 ± 0.0033	0.2505 ± 0.0014	0.3407 ± 0.0004
EXPHORMER	0.6455 ± 0.0050	0.2514 ± 0.0011	0.3501 ± 0.0013
EXPHORMER+EDGERWSE	0.6502 ± 0.0035	0.2509 ± 0.0007	0.3518 ± 0.0007
EXPHORMER+HODGE1LAP	0.6553 ± 0.0054	0.2508 ± 0.0012	0.3540 ± 0.0008

Table 3: Experiments on synthetic datasets (ACC \uparrow). The backbone model is GINE, which is not more expressive than 1-WL.

PE/SE	EXP	SR25
NONE	50	6.67
HODGE1LAP(EIGENVALUES)	100	100
EDGERWSE(FULL)	100	100