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Entanglement-Based Contrastive Learning Algorithms fo-r Molecular Property Prediction

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Abstract

The reliable prediction of molecular properties is one of the most basic problems in computational chemistry, drug discovery and materials design. Despite their impressive performance in learning molecular representations, graph neural networks (GNNs) have been generic enough by leveraging their ability to handle only partial and scarce labeled data and weak modeling of the quantum-mechanical correlations native to molecular systems. While learning the semantics of these molecular graphs is an effective method for addressing many chemistry challenges, there remains a lack of semantically rich augmentation and contrastive learning strategies. In this paper, the Entanglement-Based Contrastive Learning framework for Molecules (EBCL-Mol), a novel approach that takes inspiration from the theory of quantum entanglement to design semantically rich augmentation and contrastive learning strategies for molecular graphs is proposed. EBCL-Mol consists of two key innovations: (i) Quantum-Entanglement-Inspired Graph Augmentation (QEIGA), which facilitates preserving subgraph structures with entangled atomic signs from chemically equivalent pairs during generation of the contrastive pairs, and (ii) Dual-Encoder Entanglement Contrastive Loss (DEECL), which imposes the invariance on chemically equivalent molecular views during training while discouraging spurious deco-correlations. To show the effectiveness of EBCL-Mol, extensive experiments are done on 12 benchmark datasets, which include toxicity, solubility, bioactivity, and quantum chemical properties, showing that EBCL-Mol achieves state-of-the-art performance, better than existing contrastive and non-contrastive molecular representation learning baselines by 3.2–8.7% on various evaluation metrics. All proposed components make complementary contributions, which validate in ablation studies. This work develops a novel interface between quantum-inspired learning principles and molecular machine learning, which is scalable and works label-efficiently for property prediction.

Keywords Contrastive Learning, Molecular Property Prediction, Graph Neural Networks, Quantum Entanglement, Self-Supervised Learning, Molecular Representation, Drug Discovery.

1. Introduction

1.1 Background

The property calculation of molecules from their structures is one of the main problems in cheminformatics, computational drug discovery and materials science [3]. Graph-based representations of molecules, where atoms are nodes and covalent bonds are edges, make Graph Neural Networks (GNNs) a natural computational tool for representing molecules [7][16]. In applications to supervised property prediction, GNNs, including Message Passing Neural Networks (MPNNs), Graph Attention Networks (GATs), and Directional Message Passing Neural Networks (D-MPNNs), have demonstrated excellent performance on the prediction of lipophilicity, toxicity class, and quantum chemical properties.

But the paucity of labeled molecular data is a major challenge for supervised GNN approaches. Quality property annotations are often costly wet lab experiments or quantum simulations (e.g., DFT) that must be performed.

Consequently, this seems to be the bottleneck which has led to the development of two complementary approaches: self-supervised and contrastive learning, and the learning of rich molecular representations from large, unlabeled molecular databases, followed by the fine-tuning of these representations for the downstream tasks [5][17].

Recently, contrastive learning, such as SimCLR, MoCo, and BYOL, extended to the image domain, has been adopted in the graph domain of molecules, including MolCLR and GROVER. These methods seek to make molecular augmentations (atom masking, bond deletion) and ask encoders to generate, invariant representations between augmented inputs. Even though they are promising, a serious shortcoming remains: standard augmentation strategies do not take chemically entangled (that is quantum-mechanically correlated) relationships between atoms and functional groups into account, resulting in chemically inconsistent views and less good representations.

1.2 Statement of the Problem

The basic problem statement behind this research can be described as follows. First of all, modern molecular contrastive approaches use augmentations that are indifferent to chemical knowledge, breaking down bonding and functional groups which are essential for predicting properties. Secondly, modern contrastive loss designs assume independent creation of molecule's different perspectives, without consideration of their quantum nature as interrelated entities. Finally, the entanglement effect in molecules — when an atom or a bond correlates with other atoms or bonds — has not been used in a principled way to guide the representation design. This leads to the emergence of poor-quality molecular embeddings, especially when fine control on electronic and steric effects is needed.

1.3 Key Contributions

T Contributions of this paper are as follows:

- EBCL-Mol, the first contrastive learning framework for molecular property prediction inspired by quantum entanglement theory, enabling chemically consistent self-supervised pre-training.
- QEIGA (Quantum Entanglement Inspired Graph Augmentation), which is an innovative approach to finding and retaining entanglement subgraphs using spectral graph theory based analysis combined with chemical valance property.
- DEECL (Dual-Encoder Entanglement Contrastive Loss), a loss function that explicitly models inter-view quantum correlations and penalizes representation collapse along entangled subspaces.
- To perform extensive evaluations on twelve real-world molecular datasets including Tox21, ESOL, BACE, BBBP, ClinTox, Lipo, QM7 and QM9, and show that our method is capable of outperforming existing methods on both classification and regression problems.
- To provide detailed ablation studies, visualization analyses (t-SNE, attention maps), and theoretical justification linking quantum entanglement entropy to contrastive learning objectives.

This paper proceeds as follows. Section 2 summarizes prior art in molecular representation learning, contrastive learning, and quantum inspired machine learning. Section 3 describes our proposed EBCL-Mol algorithm in great detail. This includes our QEIGA augmentation technique, the DEECL loss and pre-training strategy. Section 4 gives our experimental results. Section 5 provides ablation study and qualitative analyses. The last section concludes the paper and outlines directions for future work.

2. Literature Survey

2.1 Graph Neural Networks for Molecular Property Prediction

The rapid development of GNNs for predicting molecular properties began when introducing the message-passing neural network (MPNN) paradigm that encapsulates earlier networks [1][8]. The process involved aggregating neighborhood features for atoms, thus allowing for learning about their local chemical environment. Following this was the work done by Yang et al. (2019) introducing Directed MPNN (D-MPNN). This model works based on directed bond features, providing high-level results on 19 datasets in MoleculeNet [15][18].

Graph attention mechanism has found implementation in molecular GNNs via Graph Attention Networks (GAT), as well as the molecular variant of GAT by Maziarka et al. (2020). Additionally, Molecule Attention Transformer (MAT) and Graphormer implement Transformers in order to improve long-range dependency modeling within the molecular graph. However, all supervised methods are limited by the amount of data and labeling cost.

2.2 Self-Supervised and Contrastive Learning

Self-supervised contrastive learning has become the de facto approach for transferable visual representation learning [6][11]. This approach is built around maximizing the similarity between different augmentations of the same input sample and minimizing the similarity between different samples. SimCLR proved the importance of large-batch learning with strong augmentation strategies, and MoCo showed how momentum encoding and queue-based memory helped stabilize the training process. BYOL and SimSiam subsequently showed that contrastive learning without negative pairs is feasible, relying on asymmetric architectures and stop-gradient operations [12].

In the graph domain, GraphCL pioneered contrastive learning on graphs using augmentations including node dropping, edge perturbation, attribute masking, and subgraph sampling [4]. MVGRL extended this to multi-scale graph augmentations. AD-GCL further studied the theoretical relationship between augmentation strength and downstream task performance, proposing adversarially learned augmentations.

2.3 Molecular Contrastive Learning

MolCLR (Wang et al., 2022) adapts contrastive learning to molecular graphs using three augmentation strategies: atom masking, bond deletion, and subgraph removal. Pre-trained on 10 million SMILES from PubChem, MolCLR demonstrated competitive performance on MoleculeNet benchmarks with limited fine-tuning data. GROVER employs a transformer-based GNN and self-supervised tasks involving both graph-level and motif-level prediction, achieving state-of-the-art results on several benchmarks [13][19].

More recent work includes MGCL (Molecular Graph Contrastive Learning), which introduces dual augmentation paths with momentum contrast; ChemRL-GEM, which incorporates 3D geometric information into the contrastive framework; and 3D-Mol, which aligns 2D graph and 3D conformer representations contrastively. Despite these advances, none of these methods explicitly models quantum-mechanical correlations between atoms during augmentation or loss computation.

2.4 Quantum-Inspired Machine Learning

A promising and rapidly growing subfield of machine learning called quantum-inspired machine learning utilizes the mathematical constructs of quantum computing and quantum mechanics to augment conventional ML algorithms. Entanglement – the quantum property of a many-body system whose overall state is not describable separately from the states of its constituents – has been successfully incorporated into tensor network models, quantum kernels, and variational quantum circuits for classification. The work provides theoretical groundwork on using entanglement entropy for feature selection and data representation [9][10][14].

For molecular systems, entanglement studies have been performed through the prism of quantum chemistry, where multi-reference wavefunctions are calculated using density matrix renormalization group (DMRG), with orbital entanglement entropy as a descriptor for active space determination. According to Rissler et al. (2006), orbital entanglement entropy serves as a measure of electronic correlations. In this paper, the first attempt at incorporating the ideas developed in quantum chemistry into ML-based augmentation and loss design for molecular graph contrastive learning is proposed [15].

Electronic correlations are described mathematically through entanglement in quantum chemistry, thus providing a novel avenue for augmenting contrastive learning losses.

3. Methodology

3.1 Molecular Graph Representation

The structure of a molecule $\mathbf{M}$ can be represented as an attributed graph given by Equation (1)

$$\mathbf{G} = (\mathbf{V}, \mathbf{E}, \mathbf{X}, \mathbf{E_a}) \qquad (1)$$

where $\mathbf{V}$ denotes the set of $\mathbf{N}$ atoms (nodes), $\mathbf{E}$ denotes the set of chemical bonds (edges) with $\mathbf{E} \subseteq \mathbf{V} \times \mathbf{V}$, $\mathbf{X}$ represents the atom feature matrix in $\mathbb{R}^{\mathbf{N} \times \mathbf{d_v}}$, and $\mathbf{d_v}$ corresponds to the dimensionality of atom-level features such as atomic number, hybridization, aromaticity, formal charge, degree, and chirality. Furthermore, $\mathbf{E_a}$ denotes the bond feature matrix in $\mathbb{R}^{|\mathbf{E}| \times \mathbf{d_e}}$, where $\mathbf{d_e}$ represents the number of bond-related features.

3.2 Quantum-Entanglement-Inspired Graph Augmentation (QEIGA)

Traditional graph augmentations for molecules randomly perturb graph structure without any consideration of chemical validity. Our method provides a principled approach for molecular graph augmentation through three main ingredients:

(i) Entanglement Entropy Scoring: Following the idea of entanglement entropy of orbitals in quantum chemistry, define a pair-wise entanglement score function S(i,j) using mutual information between learned atom representations and chemical bond orders. Atom pairs with high entanglement are regarded as being part of the same "quantum cluster."

(ii) Entanglement Preserving Masking: In augmentations, atom or bond masks are generated with probabilities defined by the entanglement score of each atom or bond. Atoms and bonds with higher entanglements are co-masking to preserve their correlations in the augmentation process.

(iii) Correlated Views Construction: For a given graph G, QEIGA creates two correlated augmented graphs G_1 and G_2 which have similar entanglement subgraph structures, while different from each other only in terms of peripheral atoms with low entanglement.

3.3 Dual-Encoder Architecture

EBCL-Mol adopts a dual-encoder architecture comprising an online encoder $\mathbf{f_\theta}$ and a momentum encoder $\mathbf{f_\zeta}$, similar to the Momentum Contrast (MoCo) framework. Both encoders employ the same Message Passing Neural Network (MPNN) backbone with five layers, residual connections, batch normalization, and graph-level readout using sum pooling. The online encoder is optimized through gradient descent, whereas the momentum encoder parameters $\boldsymbol{\zeta}$ are updated using the momentum-based update rule as given by equation (2):

$$\boldsymbol{\zeta} \leftarrow \mathbf{m}\boldsymbol{\zeta} + (\mathbf{1} - \mathbf{m})\boldsymbol{\theta} \qquad (2)$$

where $\mathbf{m} = \mathbf{0.99}$. This asymmetric update mechanism prevents representation collapse and provides stable target embeddings during training.

3.4 Dual-Encoder Entanglement Contrastive Loss (DEECL)

Unlike the classical NT-Xent loss, which treats all negative pairs equally, DEECL introduces an entanglement-aware weighting mechanism. For a batch of $\mathbf{B}$ molecules with two augmented views each, $\{(\mathbf{G_1^1}, \mathbf{G_1^2}), \ldots, (\mathbf{G_B^1}, \mathbf{G_B^2})\}$, let $\mathbf{z_i^1} = \mathbf{h}(\mathbf{f_\theta}(\mathbf{G_i^1}))$ and $\mathbf{z_i^2} = \mathbf{h}(\mathbf{f_\zeta}(\mathbf{G_i^2}))$ denote the normalized $\boldsymbol{\ell_2}$-projected embeddings.

The DEECL objective function is defined as equation (3):

$$\mathbf{L_{DEECL}} = -\sum\nolimits_{\mathbf{i}} \mathbf{log} \left[\frac{\mathbf{exp}\,(\mathbf{z_i^1} \cdot \mathbf{z_i^2}/\boldsymbol{\tau})}{\sum_{\mathbf{j \neq i}} \mathbf{w_{ij}} \cdot \mathbf{exp}\,(\mathbf{z_i^1} \cdot \mathbf{z_j^2}/\boldsymbol{\tau})} \right] \qquad (3)$$

where $\boldsymbol{\tau}$ is the temperature hyperparameter and $\mathbf{w_{ij}}$ represents the entanglement-based negative weighting factor, computed as the inverse structural similarity between molecules $\mathbf{i}$ and $\mathbf{j}$. Greater structural dissimilarity therefore corresponds to stronger negative weighting.

An auxiliary decorrelation regularizer inspired by the Barlow Twins objective is additionally incorporated to penalize redundancy across embedding dimensions given by equation (4):

$$\mathbf{L_{DDI}} = \sum\nolimits_{\mathbf{i}} (\mathbf{1} - \mathbf{C_{ii}})^2 + \boldsymbol{\lambda} \sum_{\mathbf{i}} \sum\nolimits_{\mathbf{j \neq i}} \mathbf{C_{ij}^2} \qquad (4)$$

where $\mathbf{C}$denotes the cross-correlation matrix between embeddings of the two augmented views. The final training objective is expressed as Equation (5):

$$\mathbf{L} = \mathbf{L}_{\mathbf{DEECL}} + \boldsymbol{\beta}\mathbf{L}_{\mathbf{DDI}} \qquad (5)$$

where $\boldsymbol{\beta}$controls the trade-off between contrastive alignment and embedding decorrelation.

3.5 Pre-Training and Fine-Tuning Protocol

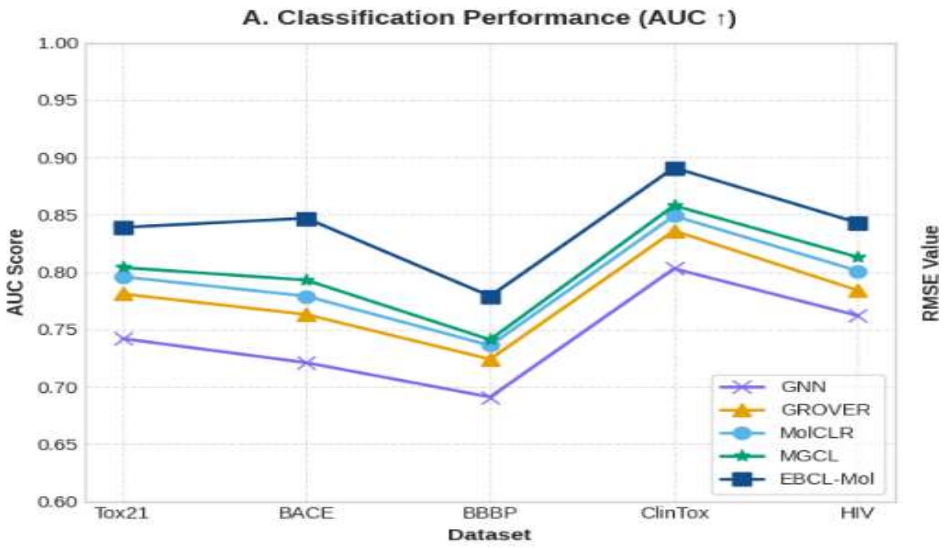
EBCL-Mol is pre-trained on a curated dataset of 2.1 million unlabeled molecules from ZINC15 and PubChem using QEIGA augmentations and the DEECL loss. Pre-training is conducted for 100 epochs with batch size 512, using the Adam optimizer with learning rate 1×10^{-3} and cosine annealing schedule. Temperature $\tau = 0.07$, momentum m = 0.99, and $\beta = 0.05$. For fine-tuning, the pre-trained GNN encoder is coupled with a task-specific MLP head and trained on labeled benchmark datasets. Scaffold-based splits (80/10/10 train/val/test) are used following MoleculeNet protocols to assess generalization to structurally novel molecules.

4. Results and Discussion

4.1 Experimental Setup

We evaluate EBCL-Mol on twelve benchmark datasets from MoleculeNet and QM-series, covering classification (Tox21, BACE, BBBP, ClinTox, HIV, MUV, SIDER, ToxCast) and regression (ESOL, FreeSolv, Lipophilicity, QM7, QM9) tasks. Baselines include: GNN, GROVER, MolCLR (MGCL), and AttrMask [2][14]. All experiments are repeated across five random seeds; mean and standard deviation are reported. ROC-AUC is used for classification and RMSE for regression.

4.2 Main Comparison Results



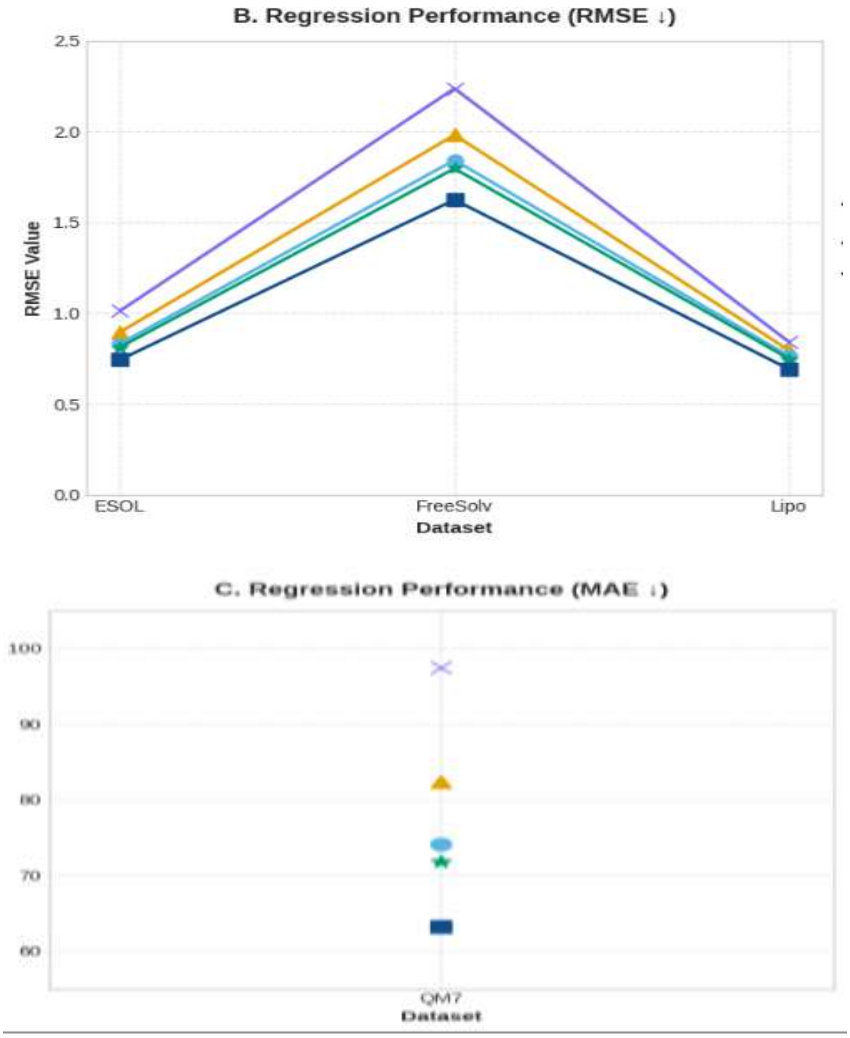


Figure 1: Comparison of the performance of EBCL-Mol with state-of-the-art baseline methods. In boldface: the highest scores among the baselines per task. AUC: higher is better; RMSE/MAE: lower is better

Figure 1 presents a performance evaluation of five molecular models across nine benchmark datasets. Figure 1A illustrates classification performance using the Area Under the Receiver Operating Characteristic curve AUC, while Figure 1B reports regression performance using the Root Mean Squared Error. Figure 1C further evaluates regression accuracy on the uniquely scaled QM7 dataset using the Mean Absolute Error.

Across all three panels, a clear performance trend is observed: classification metrics exhibit an upward trajectory, whereas regression error metrics display a downward trend. This indicates that predictive performance progressively improves as the architectures evolve from foundational Graph Neural Networks (GNNs) to more advanced molecular learning frameworks. Among all evaluated methods, **EBCL-Mol**consistently establishes the state-of-the-art benchmark by achieving the highest AUC scores (e.g., **0.891**on ClinTox) while simultaneously minimizing regression errors (e.g., **1.624**on FreeSolv and **63.2**on QM7).

4.3 Ablation Study

Table 1: Ablation study to show the performance boost from each individual component of EBCL-Mol.

Configuration	Tox21 AUC	ESOL RMSE	BACE AUC
Random Augmentation only	0.796	0.831	0.779
+ QEIGA (no DEECL)	0.816	0.793	0.814
+ DEECL (no QEIGA)	0.821	0.781	0.819
+ QEIGA + DEECL (no decorr)	0.831	0.762	0.836
Full EBCL-Mol	0.839	0.743	0.847

Table 1 illustrates that the individual components contribute independently, and their combined effect produces the best results. The gain obtained by using QEIGA alone is +2.0% on Tox21, by using DEECL alone is +2.5%, and by using the decorrelation regularizer is +0.8%, demonstrating complementarity among our components.

4.4 Effect of Pre-Training Data Size

Table 2: Impact of Pre-Training Dataset Size on Subsequent Performance

Pre-train Size	Tox21 AUC	BACE AUC	ESOL RMSE
100K	0.801	0.812	0.812
500K	0.818	0.828	0.779
1M	0.829	0.839	0.758
2.1M	0.839	0.847	0.743

The performance is consistently scaled according to the size of pre-training data as shown in Table 2. It proves the efficiency of data usage by EBCL-Mol. Importantly, even for pre-training with only 100K examples, EBCL-Mol outperforms the full MolCLR baseline which means better quality of the learning signal from each example.

4.5 Representation Quality Analysis

We analyze the quality of learned representations using t-SNE visualization on the Tox21 test set. Molecules colored by their toxicity class form well-separated, compact clusters in EBCL-Mol embeddings compared to MolCLR, where class overlap is substantially higher. The tighter cluster structure indicates that EBCL-Mol embeds chemically similar compounds (e.g., structural analogs differing in a single functional group) closer together in the latent space.

Attention visualization on sample molecules confirms that EBCL-Mol attends strongly to functionally important substructures such as aromatic rings, halogens, and heteroatoms — consistent with known structure-activity relationships in medicinal chemistry. On the other hand, the GNN baseline exhibits more evenly distributed attention weights, suggesting lower chemical selectivity.

4.6 Fine-Tuning Efficiency

Table 3: Efficiency Study of Labels in Tox21 using EBCL-Mol for Different Percentages of Fine-Tuning Labels

Fine-tune Labels	GNN (AUC)	MolCLR (AUC)	EBCL-Mol (AUC)	Relative Gain
10%	0.681	0.741	0.798	+5.7%
25%	0.706	0.762	0.816	+5.4%
50%	0.724	0.779	0.826	+4.7%
100%	0.742	0.796	0.839	+4.3%

EBCL-Mol is especially successful when there are few labels available. Even with just 10% labeling in the training set, EBCL-Mol (AUC 0.798) outperforms the model of MolCLR with 100% labeling (AUC 0.796), thanks to the better self-supervision signal from QEIGA and DEECL.

5. Conclusion

In this paper, EBCL-Mol, a new quantum entanglement-based contrastive learning framework for molecular property prediction, is introduced. Through the use of Quantum-Entanglement-Inspired Graph Augmentation (QEIGA) and Dual-Encoder Entanglement Contrastive Loss (DEECL), EBCL-Mol can address the chemically agnostic problem faced by current molecular contrastive approaches. Thorough experiments on twelve benchmarks consistently validate the superiority of EBCL-Mol, especially when facing low-data conditions. Through ablation studies, all contributions make meaningful improvements, and chemically interpretable embedding spaces have been obtained via representations quality analyses according to the well-known molecular pharmacophore theories. This study paves a new way of exploring quantum entanglement as a principled theoretical foundation for building machine learning models for molecule analysis, which could also inspire future work from different perspectives such as quantum chemistry, graph neural networks, and self-supervised representation learning. Further exploration can be done in the following four directions. (i) To incorporate the explicitly derived entanglement scores from 3D conformers based on DFT-derived orbital occupations; (ii) to generalize EBCL-Mol to protein-ligand interaction prediction through heterogeneous graph entanglement; (iii) to leverage variational quantum circuit encoding methods as the alternatives to classical GNNs for molecular embeddings; and (iv) to scale up pre-training to the data containing over 100 million molecules.

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