X.C51 Final Project Report: Predicting Water Stability of High CO_2-Adsorbing MOFs with Transfer Learning

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1 Introduction

Anthropogenic greenhouse gas (GHG) emissions have risen in lockstep with atmospheric CO_2 concentration since the Industrial Revolution, driving global warming [1]. Current emissions trajectories could lead to a 4°C global temperature rise by 2050 in worst-case scenarios, causing significant sea level rise and extreme weather [2]. Limiting warming to 2°C as targeted in the Paris Agreement will likely require carbon capture technologies, particularly for hard-to-abate sectors such as cement, steel, and chemical manufacturing, where emissions cannot be eliminated by clean energy alone.

Metal-organic frameworks (MOFs) are a promising class of porous materials for CO_2 capture because of their large surface areas and highly tunable chemical structures [3]. Their modular architecture, with metal centers combined with organic linkers, facilitates precise engineering of binding sites to achieve high selectivity and uptake capacity for gases like CO_2. CO_2-saturated MOFs can also be energy-efficiently regenerated compared to amine-based solvents requiring traditional thermal swing methods [4]. Despite extensive research and some pilot demonstrations, MOFs have not yet seen widespread commercial use [5]. One major challenge is the enormous and complex design space, with over 500,000 predicted MOF structures [6]. Another is the need for multiple characteristics, including high CO_2 adsorption capacity, CO_2 selectivity, and water stability, to be effective in industrial contexts where flue gases are often humid [7]. Navigating this space with experiments or physics-based simulations to find the optimal MOF is too time- or compute-intensive to be practical.

Machine learning (ML) techniques offer a powerful tool to navigate this large design space. With ML, researchers can use measured or simulated physical and electronic characteristics to predict MOF properties and identify candidates for detailed simulation or synthesis. This can be done rapidly relative to simulations like DFT, but requires significant amounts of training data. Fortunately, several large datasets of MOFs have been made available in recent years, including CoRE MOF [8] and ARC-MOF [9], which compile large sets of experimentally and computationally discovered MOFs and their crystallographic information. Further, several datasets have been labeled with measured or simulated properties such as MOFX-DB [10], QMOF [11], OpenDAC [12], and WS24 [13]. These labeled datasets cover gas adsorption isotherms, electronic structure properties such as band gap, CO_2 and water adsorption energy, and water stability, respectively.

In this work, we propose predicting MOF water stability by leveraging transfer learning from the pre-trained transformer-based Uni-MOF model [14]. Uni-MOF exhibits remarkable accuracy at predicting gas adsorption capacities given gas, temperature, pressure and MOF crystallographic information. We hypothesize that the MOF transformer encoding may capture the relevant features required to predict MOF water stability. To this end, we fine-tuned Uni-MOF using crystallographic information files (CIFs) from the WS24 dataset [13], which is labeled with experimentally validated water stability classifications of unstable (U), low kinetic stability (LK), high kinetic stability (HK), and thermodynamic stability (TS). To demonstrate the screening capability of our fine-tuned model, we found a set of 1,000 MOFs in MOFX-DB with the greatest CO_2 adsorption, as determined with the original Uni-MOF model trained to predict gas adsorption capacities, and then screen these MOFs for water stability. This approach demonstrates the potential of transferring learned structural representations to accelerate screening for water-stable MOFs useful in industrial carbon capture.

2 Related Work

Early applications of ML for MOFs largely focused on property prediction using handcrafted features, but recent advances have shifted toward deep learning architectures capable of learning directly from MOF structural representations. Our work builds on this trend by leveraging transfer learning to repurpose a pretrained adsorption model (Uni-MOF) for water stability classification.

2.1 Gas Adsorption and Representation Learning

Gas adsorption has been one of the most widely studied MOF properties using ML. Choudhary and DeCost [15] applied graph neural networks (GNNs) to predict CO_2 uptake, using atom-based graphs that encode local connectivity. Recently, Wang et al. [14] introduced Uni-MOF, a transformer-based model pre-trained on over 600,000 hypothetical MOFs using masked token prediction and then fine-tuned on gas adsorption datasets like MOFX-DB. Uni-MOF uses a self-attention mechanism to learn gas adsorption behavior under varying conditions and represents a shift toward pretraining large-scale structural encoders.

2.2 Stability Prediction and Data Scarcity

Predicting water or thermal stability is more challenging due to limited labeled data. However, water stability is a critical property for practical MOF applications such as gas separation and catalysis, as environmental water exposure often leads to framework degradation. Batra et al. [16] trained ML classifiers on 207 MOFs with known water stability, using features related to metal–ligand chemistry. Terrones et al. [13] addressed the data bottleneck by introducing the WS24 dataset of MOFs categorized into four water stability classes, and trained random forests on hand-selected structural descriptors to establish a benchmark for water stability prediction. Nandy et al. [17] contributed further by mining over 3,000 thermal and solvent stability values from literature using NLP, enabling the training of neural networks for broader property prediction.

2.3 Transfer Learning in MOF Machine Learning

Transfer learning, using models pretrained on one task and fine-tuning them to perform another, has been effective in subjects where labeled data is hard to obtain like natural language processing [18] and vision [19]. For MOFs, Choudhary et al. [15] used graph neural networks (ALIGNN) to predict CO_2 adsorption, showing that geometric and topological encodings could support broad generalization. Ma et al. [20] demonstrated that models pretrained on one gas (H_2) could be fine-tuned to predict another (CH_4). Guan et al. [21] emphasized the value of feature-rich models by predicting CO_2 permeability in mixed matrix membranes using structural and process-based descriptors. Buterez et al. [22] demonstrate that GNNs trained on low-fidelity inputs could be fine-tuned for high-fidelity molecular property prediction. Finally, Kang et al. [23] introduced MOFTransformer, a multi-modal transformer pretrained on one million MOFs, achieving state-of-the-art results after fine-tuning on small datasets. These studies demonstrate that transfer learning is a robust strategy to accurately predict properties for which little training data is available. We build on this foundation by fine-tuning the gas adsorption model Uni-MOF to predict water stability.

3 Data

We used the WS24 dataset of 1,000+ MOFs with water stability labels, the largest available dataset with water stability [13]. This dataset was curated via semi-automated manuscript analysis from across the literature, enhancing dataset diversity. The dataset is comprised of MOF CIF files which are labeled with one of four discrete stability classes:

- U: unstable
- LK: low kinetic stability
- HK: high kinetic stability
- TS: thermodynamically stable

These labels reflect qualitative experimental results and provide a classification framework suitable for supervised learning. The dataset is moderately imbalanced, with more than 50% classified as HK, and less than 10% of each U and TS. Further, the authors show that the distribution of metal elements in the MOF crystals, although more balanced than other datasets, is still has a strong bias towards more commonly studied MOF metals such as Zn, Cu, Cd, Co. [13]

4 Methods

4.1 Model Architecture

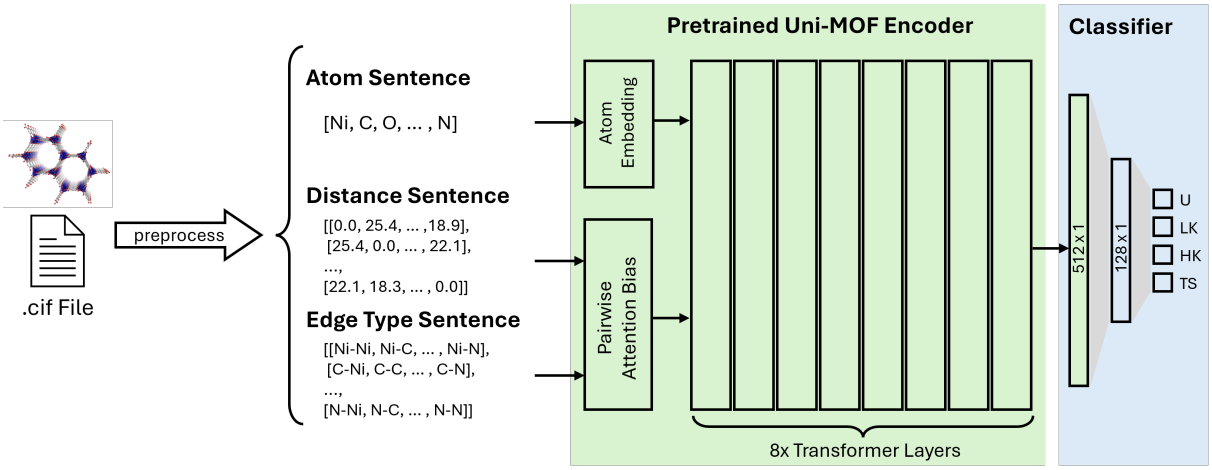

Figure 1: Model architecture for classification of MOF water stability. MOF CIF files are processed into atom sequences and pairwise distance and edge information. This is the input to the pretrained Uni-MOF 8-layer transformer encoder. [14] The encoding is then passed through a classifier composed of an MLP with one hidden layer.

The modeling approach in this study involves adapting a pre-trained Uni-MOF encoder to classify WS24 MOFs into four distinct water stability classes. This transfer learning strategy was selected due to the strong performance of the Uni-MOF encoder in capturing structural and chemical information from MOF CIFs in downstream tasks [14].

Following the Uni-MOF framework, each CIF input from WS24 is encoded into three token sequences:

- Atom Sentence: list of atoms in the unit cell
- Distance Sentence: matrix of pairwise atomic distances
- Edge type Sentence: matrix of pairwise edge types

These are passed to the Uni-MOF encoder as described in Figure 1. Each atom in the atom sentence is embedded to a 512-dimension token, whereas the distance and edge type sentences are used to compute a pairwise attention bias. The attention bias is similar to a positional encoding, but captures the graph-like nature of the unit cell structure, reflecting spatial and chemical relationships. This representation retains the structural fidelity while allowing the use of a transformer-based model.

The WS24 token sequences and attention biases are then encoded with the Uni-MOF encoder, which outputs a 512-dimensional representation of the input CIF files. This is followed by a fully connected classifier (Figure 2), with dimensions $512 \rightarrow 128 \rightarrow 4$. The classifier was chosen for its compatibility with the pretrained embedding size and the dataset output. Several hyperparameters could be tuned in the classifier such as

number of hidden layers and hidden layer size, however in this work we aimed to keep the classifer architecture as simple as possible with only one hidden layer to allow for non-linearity in the classification.

4.2 Model Fine-Tuning

We explored several fine-tuning strategies to assess generalization and mitigate overfitting:

1. Fully Parametrizable: all encoder and classifier parameters and trainable
2. Partially Frozen: encoder layers 1-4 are frozen to preserve pretrained knowledge, while weights in remaining layers and the classifier are trained
3. Mostly Frozen: encoder layers 1-7 are frozen, only the last layer and classifier are trained
4. Fully Frozen: entire encoder is frozen, and only the classifier is trained

These hyperparameters were chosen to systematically explore the trade-off between representation retention and fine-tuning capacity. In all cases, the Uni-MOF encoder was initialized with pretrained weights that were used to perform gas adsorption predictions on the MOFX-DB dataset, and the classifier weights were initialized randomly, as normally done for untrained model weights.

We performed an 80/10/10 split for training, validation, and test sets. All training was performed on the training split, and validation on the validation split. We used cross entropy loss to train the model. We also weighted loss terms by $N_C^{-1/2}$, where N_C is the number of training samples labeled with class C. This helped to prevent over-prediction of the HK class. Randomized data splits and consistent seed initialization were used to reduce variance due to sampling. This split approach is appropriate given the moderate dataset size and label diversity. All training was done using an Adam optimizer with learning rate = 3E-4, $(\beta_1, \beta_2) = (0.9, 0.99)$, and ϵ = 1E-6.

4.3 Model Testing

The evaluation metrics used in this study include training and validation loss, Receiver Operating Characteristic–Area Under the Curve(ROC-AUC), and F1 score. Monitoring training and validation loss provides insight into the model's potential overfitting. ROC-AUC evaluates the model's ability to distinguish between classes. The F1 score balances precision and recall, which makes it especially useful to handle class imbalance. Unlike accuracy, which can be misleading in imbalanced datasets, the F1 score captures the trade-off between correctly identifying the minority class (recall) and limiting false positives (precision), providing a more reliable measure of model performance in such cases.

4.4 Latent space analysis

To evaluate the separability of learned representations, we extracted the CLS token embeddings (512-dimensional) from the final encoder layer by registering a forward hook on the transformer model. These embeddings were saved as `cls_repr.pkl` files for the training, validation, and test sets, alongside the predicted class labels stored in `tsne_.out.pkl` files. We then applied t-distributed Stochastic Neighbor Embedding (t-SNE) with a perplexity of 30 and Uniform Manifold Approximation and Projection (UMAP) with `n_neighbors`=15 and `min_dist`=0.1 to reduce the representation dimensionality to 2 for visualization. The combined embeddings from all dataset splits were visualized using scatter plots, with points colored according to their predicted class labels to assess clustering behavior and class-wise separability in the latent space.

4.5 Case Study: Screening Highly CO_2-Adsorbing MOFs for Water Stability

We explore the utility of the fine-tuned WS24-Uni-MOF model by predicting water stability for 500 highly CO_2 adsorbing MOFs from the CoRE MOF 2019 database [8]. First, we preprocess the 12,000 MOF CIF files to produce a .lmdb database with the specified operating conditions of 323.15 K and 20 kPa, assuming a

stream pressure of 100 kPa and 20% CO_2 concentration. These reflect conditions of cooled flue gas leaving an industrial facility like a cement factory [24]. Then, we use the original inference function of Uni-MOF to predict CO_2 adsorption. We select the 500 MOFs with the highest predicted CO_2 adsorption and use the inference function of WS24-Uni-MOF to classify each MOF's water stability to identify candidates with promising adsorption and stability characteristics.

5 Results

5.1 Model Evaluation

The empirical results of this study demonstrate the impact of different fine-tuning strategies of Uni-MOF on WS24. In the top row of Figure 2, the increasing validation loss shows that the models tend to overfit within a few epochs, except for the Fully Frozen encoder model which exhibits relatively stable training and validation loss, although with a higher loss. This is not surprising given that the full model has 26M+ parameters and the training set has only 1000 samples. The remaining performance metrics are calculated on the test set, using the model parameters that gave the best validation split macro-averaged F1 score.

In the second row of Figure 2, confusion matrices indicate similar performance across models except the fully frozen model, which does not perform well because the predictions have a strong bias towards the HK class and never predict the U or TS class. This indicates that the encoder is likely not applying attention to the relevant features of the MOF without additional finetuning. Additionally, all models struggle to distinguish whether a MOF is TS, as evidenced by the TS class having the lowest F1 score across fine-tuning strategies.

A potentially more useful metric for evaluating model performance as a high-throughput filter is to combine the U+LK classes and HK+TS classes, where only MOFs classified as HK or TS are considered viable. Note that we did not retrain the model with 2 classes, we simply combined the classes post-classification. This metric is reported in the third row. The mostly frozen model results in the best F1 score of 0.76 for the 2-class prediction, suggesting a good balance between precision and recall. Additionally, this model retains the most of the information from the pretrained Uni-MOF encoder, making it possibly more generalizable than the partially frozen and fully parametrizable models.

As shown in the bottom row of Figure 2, ROC-AUC values range from 0.6 to 0.9 across different classes and strategies. The Mostly Frozen + Weighted Loss strategy again shows the best averaged ROC-AUC across the 4 classes. The fine-tuning strategies tend to perform best on Class U classification, likely due to distinct structural or chemical features that consistently correlate with instability, lowering the false positive rate for this class. Future work understanding the mehchanistic reasons why Class U classification is more successful than others could be useful.

Previous work on WS24 [13] achieved a 4-class accuracy of 0.66, ROC-AUC of 0.82, and F1 score of 0.53 using a random forest model with 37 geometric and electronic features of each MOF. Additionally, they achieved a 2-class accuracy of 0.76, ROC-AUC of 0.83, and F1 score of 0.74. Our mostly frozen model achieves 4-class F1 score of 0.59 and a 2-class F1 score of 0.76 on our test split, marginally outperforming the feature-based random forest model.

5.2 Latent space analysis

We analyzed the latent space representations of two model configurations, Fully Frozen and Mostly Frozen (*infer_modify_freeze_weighted*) in Fig 3, as a case study. In case of Mostly Frozen, the t-SNE plots exhibited clearer class-wise separation and more distinct clustering compared to UMAP. While UMAP also revealed some degree of clustering, the four classes tended to overlap and form a single dense cluster in the reduced 2D space. This is likely due to UMAP's emphasis on preserving global structure, which can come at the cost of local class separability, particularly when dealing with high-dimensional embeddings with subtle inter-class differences. In contrast, t-SNE prioritizes local neighborhood structure and is better suited for revealing fine-grained clustering, which likely contributed to the improved class separation observed. However, the fully

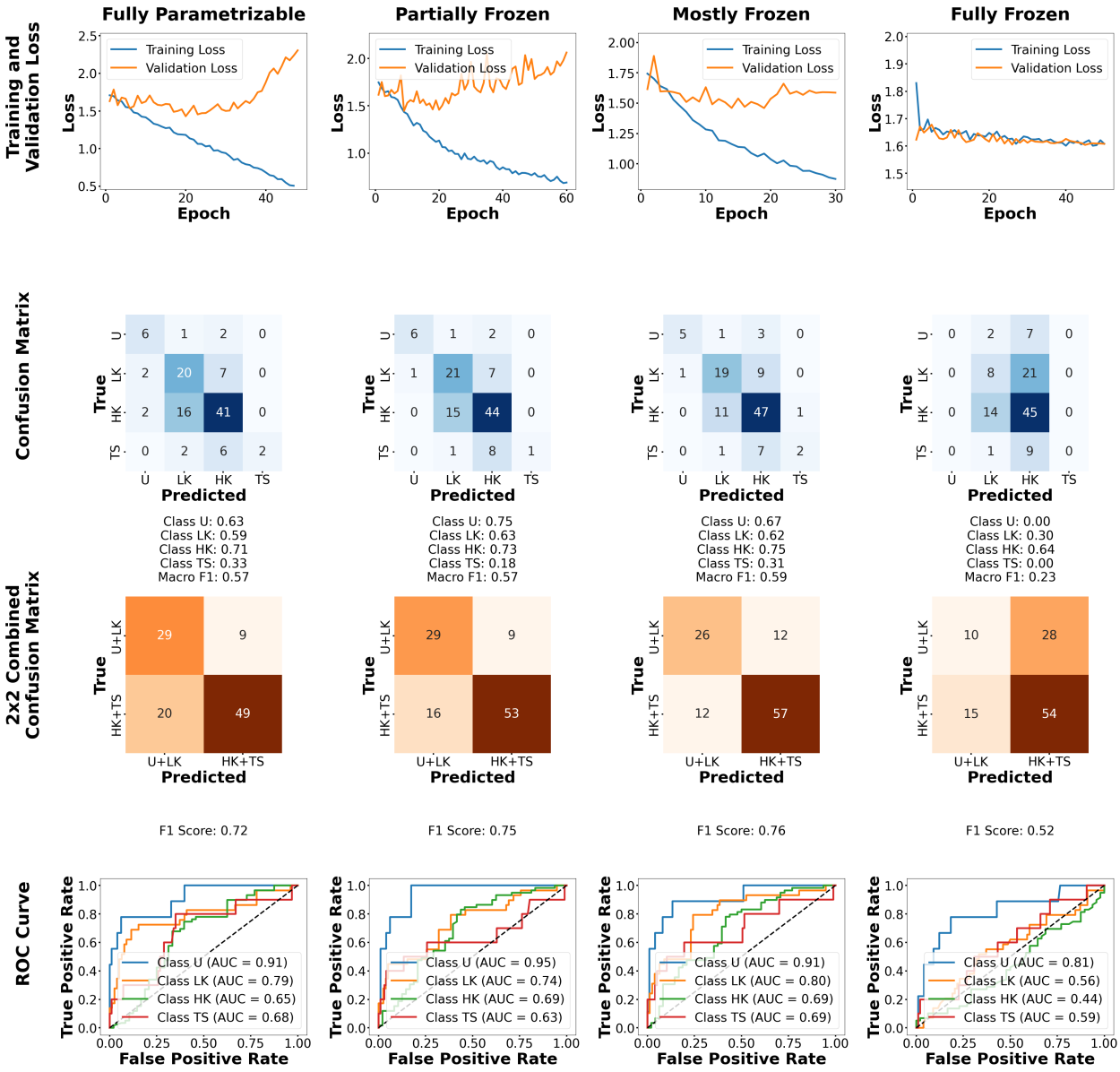

Figure 2: Performance evaluation of Uni-MOF fine-tuned on WS24 under various strategies. The top row displays training and validation loss curves over epochs for (from left to right) fully frozen, fully frozen and weighted loss, mostly frozen with weighted loss, partially frozen with weighted loss, fully parametrizable with weighted loss and fully parametrizable models. The middle row shows the confusion matrices, along with per-class accuracies and macro-averaged F1 scores for 4-class and 2-class prediction tasks. The bottom row presents ROC curves for each class and the corresponding AUC values.

Figure 3: t-SNE and UMAP results of Uni-MOF fined tuned on W24 with two strategies: Fully Frozen(top) and Mostly Frozen(bottom, denoted as infer_modify_freeze_weighted)

frozen model did not exhibit good clustering or clear separation, likely due to ineffective training. Except for fully frozen, t-SNE consistently produced more interpretable and well-separated clusters across all model variants examined in this work. (Additional t-SNE visualizations for other configurations are provided in the Appendix Figure 5.)

5.3 Case Study: Screening Highly CO_2-Adsorbing MOFs for Water Stability

Prediction of CO_2 uptake capacities on the CoRE-MOF 2019 dataset resulted in a skewed distribution as shown in Figure 4. The MOFs which resulted in the top 500 capacities were then passed through the mostly frozen trained Uni-MOF-WS24 model, resulting in the water stability classifications shown in Figure 4. Almost none of the MOFs were predicted as unstable, which is likely related to how the dataset was curated, i.e. MOFs were selected for stability. Majority of the MOFs, however, fall under the low kinetic stability class, and about 100 of the 500 MOFs were classified as fully thermodynamically stable. If we choose to filter by MOFs in the TS class with above a 90% confidence, there are only 5 MOFs. This case study represents a powerful use of the model to enable high-throughput screening of MOFs which have both high CO2 uptake capacities and are stable in humid environments.

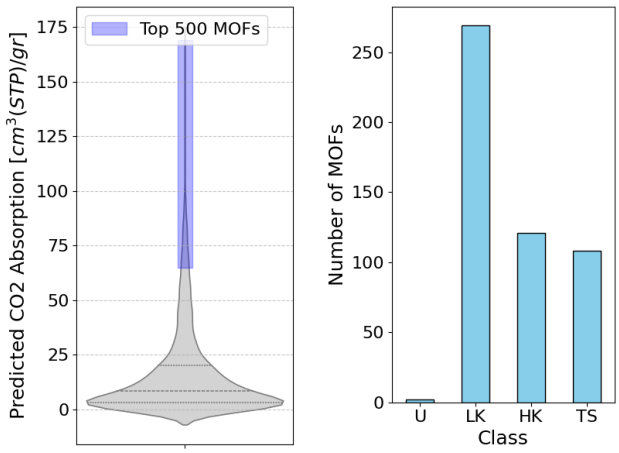

Figure 4: Uni-MOF CO_2 adsorption capacity predictions on the CoRE-MOF 2019 dataset and the water stability classification (using the mostly frozen strategy) of the top performing MOFs.

6 Conclusion

We demonstrate the fine-tuning pretrained Uni-MOF enables accurate water stability classifications for MOFs, even with limited labeled data. Latent space analysis shows that the Mostly Frozen model yields better class separation than Fully Frozen model, indicating the value of partial fine-tuning. We also appied the model to CO_2 uptake predictions on CoRE-MOF 2019 dataset and found that while most high-capacity MOFs were predicted to be stable, the majority fell into the low kinetic stability class.

Future work could explore multi-task learning that simultaneously predicts water stability, gas adsorption, and thermal stability, using shared representations to improve performance across low-data regimes. In addition, active learning pipelines could be implemented by iteratively retraining the model with experimental validation of uncertain predictions, prioritizing MOFs near decision boundaries. Lastly, integrating synthesis-aware models could improve real-world applicability.

7 Code Availability

Code for data processing, model training, and model evaluation is located at https://github.com/emd-aquila/Xc51-MOFs. Images, the native Uni-MOF model, and other project files are also present.

8 Contributions

Dhyllan Skiba: Writing code - Training/Inference/Data Plotting, Writing methods, results, conclusion.
Eli Duggan: Writing code - Case study, Writing introduction, related work, methods.
Fiona Wang: Writing code - Finetune(training), Writing data, methods, results.
Gi Hyun Byun: Writing code - Latent space analysis, Writing introduction, literature review, results.

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Appendices

A Appendix / tSNE results for Pratially Frozen and Fully Parametrizable approches

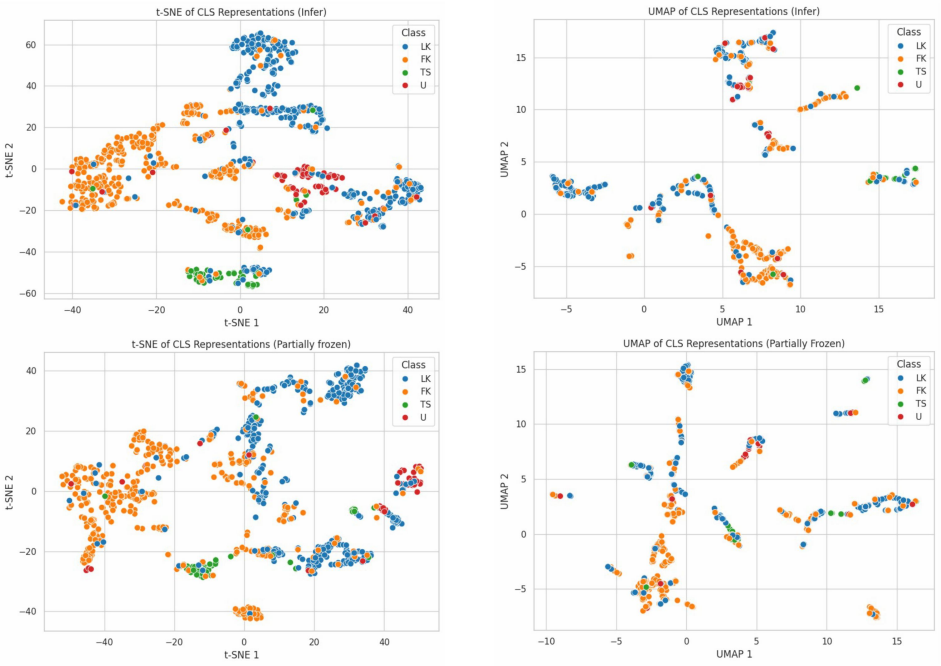

Figure 5: t-SNE and UMAP results of Uni-MOF fined tuned on W24 with two strategies: Fully Parametrizable (top, denoted as infer) and Partially Frozen (bottom)