Summary of Research at CUHK

Author: Zhizheng Zhao

🎯 1. Project Abstract

This project addresses a **fundamental theoretical limitation** in DiffCSP, a model for Crystal Structure Prediction (CSP). I first established, through theoretical analysis, that the model's reliance on **Periodic $E(3)$ Equivariance** is incomplete, as it fails to account for **Type III equivalence** arising from **Unit Cell Basis Transformations** ($\mathbf{M} \in GL(3, \mathbb{Z})$).

To achieve theoretical completeness, I proposed a **Niggli-Augmented Framework**. The core idea utilizes the **Niggli Reduction algorithm** ($\mathcal{N}$) as the mathematical tool to capture this missing Type III invariance. I designed a novel **Niggli Proxy Loss** that cleverly resolves the algorithmic non-differentiability by **decoupling** the Niggli step from the PyTorch gradient flow, effectively turning a theoretical hurdle into an engineering solution.

Preliminary experiments using a simplified MLP model successfully validated the technical feasibility of the Proxy Loss. However, a new practical bottleneck was discovered: the algorithm's **convergence failure** when processing the pathological lattices generated by the model during early training stages.

2. Motivation

The physical equivalence of crystal structures is defined by a complex manifold covering three core transformation classes. DiffCSP successfully models the first two:

Type	Equivalence Operation	Transformation Relation	DiffCSP Handling
I	External $\mathbf{O}(3)$ Rotation	$\mathbf{L}' = \mathbf{QL} \quad (\mathbf{Q} \in \mathbf{O}(3))$	**Resolved**. Handled by $\mathbf{O}(3)$-equivariant GNN.
II	Internal Periodic Translation	$\mathbf{F}' = \mathbf{w}(\mathbf{F} + \mathbf{t}) \quad (\mathbf{t} \in \mathbb{R}^3)$	**Resolved**. Handled by Fourier Features (ψ_{FT}) and the Wrapped Normal Distribution.
III	Internal Basis Transformation	$\mathbf{L}' = \mathbf{LM}, \mathbf{F}' = \mathbf{w}(\mathbf{M}^{-1}\mathbf{F}) \quad (\mathbf{M} \in GL(3, \mathbb{Z}))$	**Unresolved (Core Limitation)**. DiffCSP's features lack invariance to the $\mathbf{M}$ transformation.

DiffCSP relies on its training data having undergone strict crystallographic standardization. My analysis shows that the model is effectively learning a mapping to a single, unique standard representation, rather than learning the complete manifold of physical equivalence, thereby limiting its theoretical robustness.

3. Theoretical Framework

My core hypothesis is that a complete CSP model must integrate the handling of all symmetry groups:

- **DiffCSP ($E(3)$):** Accounts for Type I ($\mathbf{O}(3)$ rotation) and Type II (periodic translation).

- **Niggli Reduction ($\mathcal{N}$):** This is the perfect mathematical tool for Type III (basis transformation). The **Niggli reduction algorithm $\mathcal{N}$ uniquely maps all Type III equivalent lattices ($\mathbf{L}$ and $\mathbf{LM}$) to the single canonical representation $\mathbf{L}_{\text{niggli}}$**.

Therefore, a complete DiffCSP model requires an $\mathbf{O}(3)$-equivariant GNN combined with a Niggli Proxy Loss to achieve theoretical closure.

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4. Experiment

I conducted experiments on a simplified MLP model to validate the feasibility of the Niggli loss integration.

4.1 Finding 1 💡

Problem: Niggli reduction $\mathcal{N}$ is an iterative, discrete algorithm and thus **non-differentiable**. Direct loss comparison, $\mathcal{L}_{\text{loss}} = \text{MSE}(\mathcal{N}(\mathbf{L}_{\text{pred}}), \mathcal{N}(\mathbf{L}_{\text{label}}))$, breaks the PyTorch gradient flow at $\mathbf{L}_{\text{pred}}$.

My Solution (Niggli Proxy Loss): I designed a strategy to "pull" the canonical label representation into the predicted lattice's basis space, aligning the targets for a differentiable MSE calculation.

Implementation Workflow:

1. **Capture Prediction Basis:** Obtain the Niggli transformation matrix $\mathbf{N}_{\text{pred}}$ from the prediction, $\mathbf{L}_{\text{pred}}$. $(\_, \mathbf{N}_{\text{pred}}) = \text{NiggliReduce}(\mathbf{L}_{\text{pred}}.\text{detach}())$
2. **Canonicalize Label:** Obtain the canonical Niggli representation of the ground truth: $(\mathbf{L}_{\text{label,niggli}}, \mathbf{F}_{\text{label,niggli}})$.
3. **Construct Proxy Target:** Use $\mathbf{M} = \mathbf{N}_{\text{pred}}^{-1}$ (the inverse transformation) to map the canonical label into the prediction's basis:
   - **Proxy Lattice:** $\mathbf{L}'_{\text{label}} = \mathbf{L}_{\text{label,niggli}} \cdot \mathbf{M}$
   - **Proxy Coordinates:** $\mathbf{F}'_{\text{label}} = \mathbf{w}(\mathbf{M}^{-1} \cdot \mathbf{F}_{\text{label,niggli}}) = \mathbf{w}(\mathbf{N}_{\text{pred}} \cdot \mathbf{F}_{\text{label,niggli}})$
4. **Differentiable Loss Calculation:** $\mathcal{L} = \text{MSE}(\mathbf{L}_{\text{pred}}, \mathbf{L}'_{\text{label}}) + \text{MSE}(\mathbf{F}_{\text{pred}}, \mathbf{F}'_{\text{label}})$

Conclusion: The Proxy Loss successfully overcame the core non-differentiability challenge for Type III equivalence.

4.2 Finding 2 📉

Problem: Following the successful theoretical implementation, a severe practical bottleneck was encountered: the instability of the Niggli reduction algorithm.

Pathological Lattices: The untrained MLP outputs numerical unstable lattices—highly skewed, near-singular ($\det(\mathbf{L}) \approx 0$), or non-physical matrices.

Failure Mechanism: Existing tools (e.g., `spglib`) are not robust to these inputs. Their internal iterative algorithms (like the Krivy-Gruber) **fail to converge** within the maximum iteration limit, resulting in an exception (`max_iter` error).

Consequence: The failure of $\text{NiggliReduce}(\mathbf{L}_{\text{pred}}.\text{detach}())$ prevents the computation of $\mathbf{N}_{\text{pred}}$, halting the entire loss calculation and crashing the training step.

5. Conclusion and Future Work

Project Accomplishments:

1. **Theoretical Gap Identification:** Defined the missing $GL(3, \mathbb{Z})$ basis invariance in CSP models.
2. **Solution Design:** Proposed the theoretically sound Niggli-Augmented Framework.
3. **Engineering Validation:** Successfully implemented the "Niggli Proxy Loss," resolving the core non-differentiability hurdle.

Project Outlook (Next Steps):

I have successfully converted a **theoretical problem (invariance)** into an **engineering problem (algorithmic robustness)**. The immediate priority is resolving the Niggli algorithm's convergence failure in early training.