MiAD: Mirage Atom Diffusion for De Novo Crystal Generation

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Abstract

In recent years, diffusion-based models have demonstrated exceptional performance in searching for simultaneously stable, unique, and novel (S.U.N.) crystalline materials. However, most of these models don't have the ability to change the number of atoms in the crystal during the generation process, which limits the variability of model sampling trajectories. In this paper, we demonstrate the severity of this restriction and introduce a simple yet powerful technique, mirage infusion, which enables diffusion models to change the state of the atoms that make up the crystal from existent to non-existent (mirage) and vice versa. We show that this technique improves model quality by up to $\times 2.5$ compared to the same model without this modification. Mirage infusion also improves MatterGen and FlowMM, suggesting that the benefits are not limited to a single generative architecture. The resulting model, Mirage Atom Diffusion (MiAD), is an equivariant joint diffusion model for de novo crystal generation that is capable of altering the number of atoms during the generation process. MiAD achieves an 8.2% DFT S.U.N. rate on MP-20 under our evaluation protocol, the highest among the models in Table 1.

1 Introduction

Deep generative modeling opens new horizons of possibilities across various fields. Its impact is particularly profound in the natural sciences, where generative models can act as powerful exploration engines (Jumper et al., 2021) capable of dramatically accelerating scientific and technological progress. One area where this potential is especially evident is materials science. Despite the vast number of hypothetically possible materials, only a small fraction are capable of stable existence under physical constraints, the underlying principles of which remain largely unknown; this poses a significant challenge to the discovery of new materials.

Several approaches to deep generative modeling, including Generative Adversarial Networks (GANs) (Goodfellow et al., 2014; Karras et al., 2019), Variational Autoencoders (VAEs) (Kingma & Welling, 2013), Large Language Models (LLMs) (Devlin et al., 2019; Touvron et al., 2023), as well as Diffusion models (Sohl-Dickstein et al., 2015; Ho et al., 2020; Song et al., 2020; Vahdat et al., 2021) and Flow-Matching models (Lipman et al., 2022) have shown strong performance in generating complex objects. The latter two paradigms have demonstrated their potential in handling the trade-off between object quality and generation diversity (Xiao et al., 2021). These models are the same in organizing the generation process as a trainable, iterative process, which progressively refines the output over a sequence of steps.

Applying diffusion models to data from the natural sciences is non-trivial due to the need to encapsulate specific properties within a trainable dynamic framework. Multiple approaches are tailored for this objective, each addressing a particular class of properties. Currently, diffusion models can operate in non-Euclidean spaces (Huang et al., 2022; De Bortoli et al., 2022; Chen & Lipman, 2024; Okhotin et al., 2023; Hoogeboom et al., 2021) and exhibit symmetrical properties (Hoogeboom et al., 2022; Klein et al., 2023).

In recent years, diffusion models have demonstrated their potential in the domain of material science. The DiffCSP model (Jiao et al., 2023) has shown ability to generate 3D crystal structures while effectively capturing the intrinsic regularities of the crystal manifold. Additionally, the MatterGen model (Zeni et al., 2025) demonstrated that diffusion models can generate stable and novel materials – an essential quality characteristic in this task (Kazeev et al., 2025). While it is natural to expect

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generative models to generalize beyond the training data and create novel samples, this objective can sometimes conflict with the training loss, which often emphasizes fidelity to the observed data distribution. Such tension can negatively influence the model's ability to explore new regions of the data space.

However, by design, these models are restricted to generating crystals with a fixed number of atoms, which limits their ability to perform intuitive operations such as adding or removing specific atoms during generation. As we show in Section 4, this constraint reduces the model's flexibility and hinders its ability to explore a broader range of plausible crystal structures, impacting both the diversity and quality of the generated outputs.

In this paper, we present the next steps toward improving diffusion models for crystal generation and demonstrate their significance in the search for novel and stable materials:

- We propose a simple yet powerful technique, *mirage infusion*, which broadens the original space of 3D crystal structures, enabling the diffusion model to modify the number of atoms in the crystal during the generation process.
- We examine the sensitive parameters of the proposed technique and their impact on the quality of the generative model through a series of experiments.
- We demonstrate that the proposed approach significantly enhances the performance of the base joint diffusion model and achieves the highest reported S.U.N. among the models in Tables 1 and 2.

2 PRELIMINARIES

2.1 DIFFUSION MODELS

A diffusion model is a generative model that consists of forward and backward processes:

$$q(x_{0:T}) = q(x_0)\prod_{t=1}^{T} q(x_t|x_{t-1}), \qquad p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t),$$

where $q(x_0)$ represents the data distribution, $q(x_t|x_{t-1})$ denotes the transition kernel which gradually adds noise to data objects, $p(x_T)$ is the prior distribution from which the diffusion model begins generation, and $p_\theta(x_{t-1}|x_t)$ is the trainable transition kernel used for step-by-step object denoising during the sampling procedure. The original training objective for the backward process is the Evidence Lower Bound (ELBO). Alternatively, in continuous spaces, diffusion models can be reformulated using *score-matching*. In this framework, the model is trained using the *conditional score* $\nabla_{x_t} \log q(x_t|x_0)$ which allows it to approximate the *unconditional score* $\nabla_{x_t} \log q(x_t)$ required for sampling.

Finally, for data with complex internal structures, one can factorize objects into several components and define a separate diffusion process for each of them. As an example, crystals can be factorized into three components: lattice matrix, fractional coordinates of atoms and atom types, where each component belongs to a space with a specific geometry that differs from the others. In the model, which we extend in this work, the crystal structure is decomposed into a lattice matrix, fractional atomic coordinates, and atom types – each residing in a space with distinct geometric properties. In this setting, the sampling procedure requires simultaneous denoising of all these components. Therefore, we can use a single neural network, which takes the noisy versions of all object components and denoises them according to their respective diffusion processes. In this way, the diffusion model for each component is conditioned on the noisy versions of all object components forming a *joint diffusion model*. The resulting training objective is a weighted sum of the objectives from all diffusion processes.

2.2 CRYSTAL REPRESENTATION

The representation of a 3D crystal can be reduced to the representation of a *unit cell*, with the entire crystal being an infinite repetition of its unit cell. A unit cell is represented by the lattice

$L = [l_1, l_2, l_3] \in \mathbb{R}^{3\times3}$ – three basis vectors that define its geometry, $F \in [0,1)^{N_{\text{atoms}}\times3}$ – the fractional coordinates of atoms within the unit cell, and $A \in \{1,\dots,N_{\text{types}}\}^{N_{\text{atoms}}}$ – the types of atoms. The number of atoms in the unit cell, $N_{\text{atoms}} \in \mathbb{N}_+$, varies depending on the specific crystal. The entire crystal is an infinite periodic structure, defined as a set of atoms given by:

$$\{(a_i, x_i) \mid x_i = (f_i + k)L,\ \forall k \in \mathbb{Z}^3\},$$

where each atom is represented by a pair consisting of its type a_i and its Cartesian coordinates x_i. Thus, the task of generating a crystal reduces to generating the triplet $\mathcal{M} = (L, F, A)$.

2.3 Diffusion model for crystals

The joint diffusion model over crystal structures $\mathcal{M} = (L, F, A)$ is proposed in Jiao et al. (2023); Zeni et al. (2025). In this model, the forward process is factorized across the lattice L, fractional coordinates F, and atoms types A:

$$q(\mathcal{M}_t|\mathcal{M}_{t-1}) = q(L_t|L_{t-1})q(F_t|F_{t-1})q(A_t|A_{t-1}),$$

where $\mathcal{M}_0 = (L_0, F_0, A_0)$ denotes a clean crystal, while $\mathcal{M}_t = (L_t, F_t, A_t)$ represents an intermediate noisy version of the crystal.

2.3.1 Diffusion components

Lattice Given that $L_0 \in \mathbb{R}^{3\times3}$, we can employ DDPM (Ho et al., 2020) with Gaussian distributions:

$$\begin{aligned} q(L_t|L_{t-1}) &= \mathcal{N}\left(L_t|\sqrt{\beta_t}L_{t-1}, \sqrt{1-\beta_t}I\right), \\ p(L_T) &= \mathcal{N}\left(L_T|0, I\right), \\ p_\theta(L_{t-1}|\mathcal{M}_t) &= \mathcal{N}\left(L_{t-1}|\mu_\theta(\mathcal{M}_t, t), \sigma_t^2 I\right), \end{aligned}$$

where $\beta_t \in \mathbb{R}_+$ – sets the scale of noise for step t and $p_\theta(L_{t-1}|\mathcal{M}_t)$ is conditioned on the noisy versions of all crystal components, as it is a joint diffusion model. The training objective for this diffusion component is defined as a weighted ELBO, which reduces to the following form:

$$\mathcal{L}_L = \sum_{t=2}^{T} \gamma_t \mathbb{E}_{\mathcal{M}_0\sim q(\mathcal{M}_0), \mathcal{M}_t\sim q(\mathcal{M}_t|\mathcal{M}_0)} \text{KL}\left[\, q(L_{t-1}|L_t, L_0) \,||\, p_\theta(L_{t-1}|\mathcal{M}_t)\,\right].$$

Fractional coordinates The space of fractional coordinates is periodic. Therefore, we need to utilize a diffusion model that can accommodate data of this nature. One possible option is to use a Wrapped Normal distribution for each coordinate of each atom:

$$\begin{aligned} q(F_t|F_{t-1}) &= \mathcal{WN}\left(F_t|F_{t-1}, (\sigma_t^2 - \sigma_{t-1}^2)I\right), \\ p(F_T) &= \mathcal{U}\left(F_T|0,1\right), \end{aligned}$$

where $\sigma_t \in \mathbb{R}_+$ – set the scale of noise for step t. A particularly suitable and efficient method for training the backward process in this model is to adopt Riemannian score matching (De Bortoli et al., 2022) with the following objective:

$$\mathcal{L}_F = \mathbb{E}_{\mathcal{M}_0\sim q(\mathcal{M}_0), t\sim\mathcal{U}(1,T), \mathcal{M}_t\sim q(\mathcal{M}_t|\mathcal{M}_0)} ||\nabla_{F_t} \log q(F_t|F_0) - s_\theta(\mathcal{M}_t, t)||_2^2,$$

where s_θ is a neural network that approximates the unconditional score for the generating procedure proposed by Jiao et al. (2023).

Atom types The atom type is a discrete variable drawn from a fixed set of N_{types} possible elements. We use D3PM (Austin et al., 2021) for this component:

$$\begin{aligned} q(A_{t,i}|A_{t-1,i}) &= \text{Cat}\left(A_{t,i}|Q_t A_{t-1,i}^{\text{onehot}}\right), \\ p(A_{T,i}) &= \text{Cat}\left(A_{T,i}|\mathbf{1}/N_{\text{types}}\right), \\ p_\theta(A_{t-1,i}|\mathcal{M}_t) &= \text{Cat}\left(A_{t-1,i}|c_{\theta,i}(\mathcal{M}_t, t)\right), \end{aligned}$$

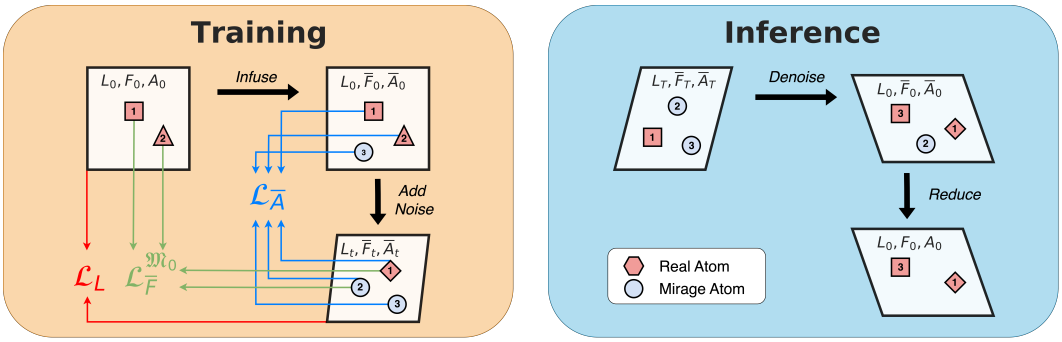

Figure 1: Overview of the proposed mirage infusion technique.

where $A_{t,i}$ – the atom type of atom i in the crystal $\mathcal{M}_t$, $A^{\text{onehot}}_{t-1,i}$ – zero vector of size N_{types} with 1 on position $A_{t-1,i}$, $\mathbf{1}$ – unit vector of size N_{types}, $Q_t \in \mathbb{R}_+^{N_{\text{types}} \times N_{\text{types}}}$ – matrix that gradually spreads probability mass across all types on each step t, $c_{\theta,i}$ – prediction of probabilities of each type for atom i. The training objective takes the following form:

$$\mathcal{L}_A = \sum_{t=2}^{T} \mathbb{E}_{\mathcal{M}_0 \sim q(\mathcal{M}_0), \mathcal{M}_t \sim q(\mathcal{M}_t|\mathcal{M}_0)} \sum_{i=1}^{N_{\text{atoms}}} \text{KL}\left[\, q(A_{t-1,i}|A_{t,i}, A_{0,i}) \;||\; p_\theta(A_{t-1,i}|\mathcal{M}_t) \,\right].$$

Although the model is capable of generating crystals with different numbers of atoms, this number must be specified before the generation process begins.

The final objective for this joint diffusion model is a weighted sum of the objectives for the components L, F, and A:

$$\mathcal{L} = \kappa_1 \mathcal{L}_L + \kappa_2 \mathcal{L}_F + \kappa_3 \mathcal{L}_A \to \min_\theta,$$

where the coefficients $\kappa_i > 0$ for $i = 1, 2, 3$ affect component prioritization, provided that we use the same neural network for making predictions.

2.3.2 Invariances

The joint diffusion model outlined in the previous section is applied within the domain of crystals, which possesses distinct properties referred to as *symmetries*. To ensure these symmetries are preserved, the model must be parametrized in a particular manner. Further details regarding the specific types of symmetries present in the domain of crystals, as well as the organization of diffusion components required to achieve invariance to these symmetries, are provided in Appendix A.

3 Mirage Infusion

Motivation In the joint diffusion model, the number of atoms in a crystal N_{atoms} must be fixed in advance during the generation procedure to sample $\mathcal{M}_T$ from the prior distribution:

$$\mathcal{M}_T \sim\; p(\mathcal{M}_T|N_{\text{atoms}}) = p(L_T, F_T, A_T|N_{\text{atoms}}) = p(L_T)p(F_T|N_{\text{atoms}})p(A_T|N_{\text{atoms}}), \qquad (1)$$

where N_{atoms} is typically drawn from a categorical distribution $p(N_{\text{atoms}})$, estimated from the training data (Jiao et al., 2023), and it usually spans a limited range of discrete values (e.g., 1 to 20). Consequently, the number of atoms in a crystal's unit cell is fixed during the whole process of generation, which, as we show in the following sections, crucially limits the model's flexibility. To address this limitation, we introduce a framework that supports adding or removing atoms during generation.

Core idea A wide subset of diffusion models for crystalline materials cannot change the number of atoms during generation. To enable this, we reinterpret the addition and removal of atoms as

transitions between different types of atoms. Specifically, we introduce *mirage atoms* – placeholder atoms that may either materialize into real atoms or vanish during the generation process.

In a crystal representation $\mathcal{M}$, mirage atoms are distinguished by assigning them a special type. Since F is continuous, it cannot be used to flag mirage atoms directly. However, A is discrete, so we designate a new atom type 0 to represent a mirage atom.

Method To support mirage atoms, we define an *expanded crystal domain* $\overline{\mathcal{M}} = (L, \overline{F}, \overline{A})$, where all objects have a fixed number of atoms N_{m} that is greater than or equal to the maximum number of atoms in a crystal in the training dataset. Mirage atoms are simply atoms with type 0 in this domain.

We define two mappings:

- **Infusion**: Adds mirage atoms to a real crystal $\mathcal{M}$. The original atoms are kept unchanged, while the additional atoms are initialized with type 0, and fractional coordinates are drawn from the uniform distribution over the unit cell $\mathcal{U}(0,1)^3$.
- **Reduction**: Removes mirage atoms from expanded crystal $\overline{\mathcal{M}}$ by filtering out all atoms with type 0, restoring the original representation $\mathcal{M}$.

Using this setup, we can train a diffusion model in the expanded domain. The model architecture remains nearly the same, with the only change being an extra atom type (type 0) in the D3PM diffusion component for atom types.

Algorithm 1 MiAD Training

1: **repeat**
2: Sample $t \sim \mathcal{U}(1, T)$
3: Sample $\mathcal{M}_0 \sim q(\mathcal{M}_0)$
4: Infuse mirage atoms $\mathcal{M}_0 \to \overline{\mathcal{M}}_0$
5: Add noise $\overline{\mathcal{M}}_t \sim q(\overline{\mathcal{M}}_t|\overline{\mathcal{M}}_0)$
6: Minimize $\kappa_1\mathcal{L}_L + \kappa_2\mathcal{L}_{\overline{F}}^{\mathfrak{M}_0} + \kappa_3\mathcal{L}_{\overline{A}}$
7: **until** Convergence

Algorithm 2 MiAD Sampling

1: Sample $\overline{\mathcal{M}}_T \sim p(\overline{\mathcal{M}}_T)$
2: **for** $t \leftarrow T$ **to** 1 **do**
3: Denoise $\overline{\mathcal{M}}_{t-1} = p_\theta(\overline{\mathcal{M}}_{t-1}|\overline{\mathcal{M}}_t)$
4: **end for**
5: Reduce $\overline{\mathcal{M}}_0 \to \mathcal{M}_0$

In training, crystal from the training data $\mathcal{M}_0$ is infused with the mirage atoms with randomly initialized fractional coordinates, effectively augmenting the dataset. The lattice loss remains unchanged. The atom-type loss remains the same as well, training the model to predict real and mirage atom types in the final structure. For fractional coordinates loss, we ignore the mirage atoms by defining a mask $\mathfrak{M}_0 = \{i \mid \overline{A}_{0,i} \neq 0,\ i = \overline{1, N_{\text{m}}}\}$ for the original crystal $\mathcal{M}_0$, since they have no ground-truth positions. This allows the model to freely adjust their positions and focus learning only on real atoms. The loss is masked accordingly:

$$\mathcal{L}_{\overline{F}}^{\mathfrak{M}_0} = \mathbb{E}_{\overline{\mathcal{M}}_0 \sim q(\overline{\mathcal{M}}_0), t \sim \mathcal{U}(1,T), \overline{\mathcal{M}}_t \sim q(\overline{\mathcal{M}}_t|\overline{\mathcal{M}}_0)} \sum_{i \in \mathfrak{M}_0} ||\nabla_{\overline{F}_{t,i}} \log q(\overline{F}_t|\overline{F}_0) - s_{\theta,i}(\overline{\mathcal{M}}_t, t)||_2^2, \quad (2)$$

where $q(\overline{\mathcal{M}}_0)$ is a distribution of crystals after the infusion of mirage atoms, and $s_{\theta,i}(\overline{\mathcal{M}}_t, t)$ is a score for the fractional coordinates of atom i.

The sampling algorithm remains the same, except for two differences: (1) at the start of generation, all crystals are sampled with the same number of atoms N_{m} (not with $N_{\text{atoms}} \sim p(N_{\text{atoms}})$ as in 1), (2) at the end of generation we need to apply the reduction operator to project the crystal onto the original domain.

Importantly, this method preserves existing symmetries because lattice representations remain unchanged and mirage atoms follow the same spatial rules as real atoms.

We call the proposed technique *mirage infusion*. It expands the space of generative trajectories available to the model, increasing its flexibility and expressiveness. We outline the training procedure in Algorithms 1, and the sampling procedure in Algorithm 2, as well as their schematic visualization in Figure 1.

Discussion We review existing generative models for crystals and their treatment of the number of atoms in Appendix C. There are several design choices when defining the expanded domain. In our setup, we: (1) initialize mirage atoms with uniformly random coordinates. This choice ensures that mirage atoms can occupy arbitrary positions in the unit cell and introduces variability into the generation process. (2) Mask the loss for mirage atoms during training to avoid learning from noise.

This allows the model to focus on denoising atoms that exist in the final structure while giving it the freedom to learn when and how mirage atoms should transform into real ones during generation. Skipping the mask would force the model to predict a zero score for mirage atoms, potentially reducing expressiveness.

A similar idea was independently proposed by Schneuing et al. (2025) for structure-based drug design. In their method, mirage atom coordinates are initialized at the object's center of mass, and no loss masking is applied. In Appendix B.3 we demonstrate that this technique fails to work for de novo crystal generation, underscoring the significance of our proposed design choices.

4 Experiments

De novo crystal generation serves as the first step of the material discovery pipeline. In our experimental evaluation, we aim to highlight the importance of the model's capability to modify the number of atoms during the generative process. The proposed approach is a combination of the DiffCSP model Jiao et al. (2023) with the proposed mirage infusion technique (see Section 3). To isolate the effect of this technique, we retain an identical neural network architecture, thereby minimizing confounding variables.

Evaluation protocol Among existing approaches for comparing generative models in de novo crystal generation, we focus on S.U.N. that was firstly proposed in Zeni et al. (2023) and was used in multiple works (Miller et al., 2024; Levy et al., 2025; Sriram et al., 2024; Kazeev et al., 2025; Joshi et al., 2025). S.U.N. is a proportion of materials that are simultaneously *stable*, *unique* and *novel*. A detailed explanation of this metric presented in Appendix D. This is one of the most reasonable measures of a generative model's performance, as it directly quantifies the model's utility for materials discovery. It should be noted that comparisons based solely on the stability rate or solely on the uniqueness-and-novelty rate are not meaningful, because both metrics can be easily gamed – by overfitted models and by random generative models, respectively. Main experiments are conducted using the MP-20 dataset (Jain et al., 2013), and results are assessed using various versions of the S.U.N. metric. Details of the experimental setups are provided in Appendix G. Xie et al. (2021) proposed several metrics for evaluating generative models in this task: Structural and Compositional Validity, Coverage-Recall, Coverage-Precision, and Wasserstein distances between the distributions of various properties in the training set and those of crystals produced by the model. Although these metrics have become widespread tools for model comparison, they have severe limitations that constrain their applicability to analyzing the performance of modern generative models. These limitations were already outlined in Sriram et al. (2024), De Breuck et al. (2025). We report MiAD's results under these metrics, as well as our arguments against their use in their current form, in Appendix E.

Design choices Appendix B provides a detailed exposition of the key design choices underlying the mirage infusion technique. To begin with, we show that the proposed technique is robust to a non-optimal choice of its sole hyperparameter, N_{m}, defined as the total number of real and mirage atoms for crystals in the expanded domain (see Appendix B.1). We further observe that the loss in joint diffusion models is sensitive to the relative weighting of the losses from each diffusion component. Because mirage infusion affects the scaling of the loss terms associated with fractional coordinates and atom types, we run additional experiments to remove this confounding factor and ensure a fair comparison (see Appendix B.2). In all subsequent experiments, we preserved the same balance between loss components and did not tune it. As discussed in Appendix C, alternative formulations of mirage infusion have been proposed. We compare

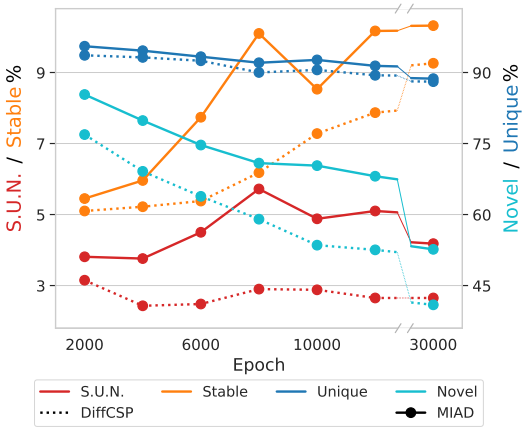

Figure 2: Comparison of MiAD (DiffCSP with mirage infusion) and DiffCSP in terms of stability, uniqueness, novelty, and S.U.N. Stability is estimated via eq-V2.

Table 1: **Crystal generation comparison via S.U.N. based on DFT.** We report metastability, M.S.U.N., stability, and S.U.N. for 10 000 sampled crystals. For clarity in evaluating the model's quality, we also report the Unique&Novel rate separately for metastable and stable crystals, respectively. MiAD outperforms all existing approaches in terms of M.S.U.N. and S.U.N. DiffCSP & FlowMM results are taken from Miller et al. (2024), FlowLLM Sriram et al. (2024), ADiT Joshi et al. (2025); WyFormer computed by us from the DFT structures provided by the authors.

Model	Metastability ($E^{\text{hull}} < 0.1$)			Stability ($E^{\text{hull}} < 0.0$)		
	Metastable (%)	Unique&Novel (%)	M.S.U.N.↑ (%)	Stable (%)	Unique&Novel (%)	S.U.N.↑ (%)
DiffCSP	-	-	-	5.0	66.0	3.3
FlowMM	30.6	73.5	22.5	4.6	60.9	2.8
FlowLLM	66.9	39.3	26.3	13.9	33.8	4.7
WyFormer	30.5	89.8	27.4	5.2	92.3	4.8
MP20-only ADiT	71.1	53.6	38.1	12.8	50.8	6.5
Jointly trained ADiT	81.0	34.8	28.2	15.4	34.4	5.3
MiAD	73.5	59.4	**43.6**	12.5	65.2	**8.2**

Table 2: **Crystal generation comparison via S.U.N. based on MLIPs.** We report stability and S.U.N. estimated using CHGNet and eq-V2 for 10 000 sampled crystals. For clarity in evaluating the model's quality, we also report the Unique&Novel rate among stable crystals. MiAD achieves the highest S.U.N. under both CHGNet and eq-V2 in this comparison. All results are computed under our MP-20 S.U.N. protocol on structures sampled from the official repositories or author-released checkpoints of each model.

Model	eq-V2 ($E^{\text{hull}} < 0.0$)			CHGNet ($E^{\text{hull}} < 0.0$)		
	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)
CDVAE	-	-	-	4.4	96.4	4.3
DiffCSP	3.8	66.6	2.5	11.3	78.8	8.9
DiffCSP++	2.9	73.5	2.1	11.4	75.9	8.6
FlowMM	2.0	70.4	1.4	9.1	71.7	6.5
SymmCD	2.8	70.3	2.0	9.3	73.5	6.9
SymmBFN	-	-	-	11.8	75.4	8.9
MatterGen MP-20	2.5	73.6	1.8	9.7	83.5	8.1
CrystalDiT	3.8	83.1	3.1	19.6	63.0	12.3
Crystalite	6.3	66.9	4.2	15.2	72.2	11.0
OMatG	1.0	36.1	0.4	8.2	48.3	4.0
MiAD	9.7	56.7	**5.5**	19.8	65.2	**12.9**

our definition against a contemporary variant and demonstrate the latter's inapplicability to de novo crystal generation (see Appendix B.3). This highlights the critical importance of the design of the expanded domain and the modifications to the loss function. Finally, in Figure 2, we contrast the final variant of Mirage Infusion with the baseline model – lacking these modifications – across a range of training budgets. The results demonstrate that the substantial gains achieved by the proposed method, concurrently in terms of stability, uniqueness, and novelty rate, cannot be attributed merely to the allocation of additional computational resources. This ablation is performed using S.U.N., where stability is estimated using eq-V2 (Barroso-Luque et al., 2024) due to computational constraints.

Main comparisons We designate the finalized model as MiAD (Mirage Atom Diffusion) and benchmark its performance against state-of-the-art methods for de novo crystal generation. Multiple versions of the S.U.N. metric are employed to facilitate comprehensive comparisons across a broad range of existing models. It should be noted that we do not compare against studies that lack S.U.N. metric evaluations.

Table 3: **Transferability of mirage infusion across joint (L, F, A) generators.** We report CHGNet M.S.U.N. and S.U.N. for 10 000 sampled crystals on MP-20. For each backbone, the baseline is independently reproduced and mirage infusion is applied under an otherwise identical training and sampling configuration. MatterGen and FlowMM baselines may therefore differ from the literature values in Table 2. Mirage infusion yields consistent gains on both diffusion (DiffCSP, MatterGen) and flow-matching (FlowMM) models.

Model	M.S.U.N. ↑ ($E^{\text{hull}} < 0.1$)		S.U.N. ↑ ($E^{\text{hull}} < 0.0$)	
	Baseline (%)	+ Mirage Infusion (%)	Baseline (%)	+ Mirage Infusion (%)
DiffCSP	52.4	**55.9**	8.9	**12.9**
MatterGen	47.1	**52.6**	6.1	**10.4**
FlowMM	42.9	**47.1**	7.0	**10.2**

Comparison in Table 1 presents the results, demonstrating MiAD performance against existing approaches, with respect to the S.U.N. metric, where stability is assessed via DFT (Kohn & Sham, 1965) according to the protocol described in Appendix F. As outlined in Appendix D, this configuration represents the most rigorous S.U.N. evaluation and currently prevails over all other approaches. While MiAD exhibits a lower fraction of stable crystals compared to ADiT (Joshi et al., 2025), this is attributable to the tendency of this model to replicate training set samples. This can be seen by comparing ADiT and MiAD in terms of the uniqueness and novelty rates among stable crystals, reported in the Unique&Novel column of Table 1. Consequently, stability alone is insufficient as a measure of generative model quality. At the same time, MiAD exhibits a lower fraction of unique and novel crystals among stable compared to WyFormer, while exceeding the last one in terms of stability rate. Therefore, MiAD achieves superior overall S.U.N. performance relative to all baselines ($+25\%$ relative to the closest competing method) due to the best trade-off between stability, uniqueness, and novelty. Another significant observation is that the incorporation of mirage infusion enhances the performance of the original DiffCSP model by up to $\times 2.5$ times, representing a substantial improvement.

Furthermore, some works only report S.U.N. computed with MLIPs, presumably due to computational constraints. Table 2 shows that MiAD achieves the highest S.U.N. under both MLIPs in our evaluation. CrystalDiT (Yi et al., 2026) reports strong S.U.N. under DFT, but its evaluation protocol first filters for uniqueness and novelty, then prerelaxes the remaining structures and estimates stability on that subset. In our evaluation, $\approx$11.6% of crystals from CrystalDiT that are novel before prerelaxation are no longer novel after prerelaxation, which inflates reported novelty and S.U.N. MiAD remains ahead on eq-V2 S.U.N. (5.5% vs. 3.1%). Crystalite (Hadži Veljković et al., 2026) ranks highly on LeMat-GenBench (Betala et al., 2025), which measures novelty against LematBulk, a much larger reference than MP-20. Penalizing MP-20-trained models for generating structures outside MP-20 but inside LematBulk is therefore a poor match for comparing generative-model design, and we report Crystalite under MP-20 novelty. OMatG (Höllmer et al., 2025) is included as an additional MP-20 baseline.

Transferability The comparisons above isolate the effect of mirage infusion on the DiffCSP backbone. To test whether these gains transfer beyond this architecture, we apply the same technique to MatterGen (Zeni et al., 2025) and FlowMM (Miller et al., 2024), which share the (L, F, A) representation and the corresponding factorization of the loss. For each backbone we independently reproduce the baseline and infuse mirage atoms under an otherwise identical training and sampling configuration. Table 3 reports CHGNet M.S.U.N. and S.U.N. on MP-20. Mirage infusion raises CHGNet S.U.N. from 8.9% to 12.9% for DiffCSP, from 6.1% to 10.4% for MatterGen, and from 7.0% to 10.2% for FlowMM. The same pattern holds for metastability: M.S.U.N. increases from 52.4% to 55.9%, 47.1% to 52.6%, and 42.9% to 47.1%, respectively. These results confirm that the improvement is not DiffCSP-specific and that mirage infusion transfers to both diffusion and flow-matching models in this paradigm.

Scalability The proposed model incurs higher computational costs due to the increased average number of atoms per generated crystal. Additionally, mirage infusion requires more optimization

iterations to achieve optimal performance. Details about computational overhead are provided in Appendix G.5. Experiments demonstrating the scalability of the proposed method to tasks with a higher maximum number of atoms are conducted on the MPTS-52 dataset and provided in Appendix H. There, we also introduce MiAD-WRNA, a dynamic mirage sampling that substantially mitigates the computational overhead, reducing the training time multiplier from $\times 2.26$ to $\times 1.14$ relative to the baseline, while preserving quality improvements. Finally, the scalability of the proposed model on larger datasets is demonstrated in Appendix I, where we evaluate MiAD on the large-scale Alex-MP20 dataset (Zeni et al., 2025). We show that MiAD successfully scales to this broader distribution without additional hyperparameter tuning, achieving SOTA performance.

Additional analyses We investigated the generative behavior and diversity of MiAD. In Appendix J, we analyze the distribution of atom counts, confirming that MiAD actively varies the number of atoms during generation and successfully produces S.U.N. crystals across a wide range of sizes. In Appendix K, we examine the spacegroup distributions of modern generative models, demonstrating that MiAD preserves structural diversity without suffering from mode collapse, effectively generating crystals across various symmetry families. Finally, in Appendix L we provide a qualitative demonstration illustrating how MiAD uses mirage atoms when generating a particular crystal. Specifically, we show that this mechanism functions as an active error-correction system: the model dynamically prunes structurally disadvantageous atoms and completes missing lattice components on the fly to escape poor local minima, restore symmetries, and achieve thermodynamic stability.

5 Discussion

Conclusion The categorization provided in Appendix C offers valuable insights into the potential applicability of the proposed technique across a range of models within the domain of de novo material generation. Beyond DiffCSP, which serves as the foundation for the model introduced in this work, the mirage infusion technique can be directly implemented, without modification, in MatterGen, FlowMM, and CrystalFlow, given that these models employ an identical crystal representation and share the same factorization of the loss function. We empirically confirm this transfer for MatterGen and FlowMM in Section 4. Additionally, we hypothesize that an adapted version of this technique could be extended to models such as ADiT, CDVAE, FlowLLM, SymmCD, and SymmBFN, although further investigation is required to assess its effectiveness, and the eventual impact in these cases remains uncertain. At the same time, we present MiAD, demonstrating that mirage infusion gives a substantial boost in quality for the base joint diffusion model and achieves the highest S.U.N. among the models evaluated in Tables 1 and 2. This improvement demonstrates the potential of approaches directed at the modification of the space with which a particular diffusion model works.

Societal impact Mirage Atom Diffusion improves the diversity and quality of generated materials and may accelerate discovery in clean energy, electronics, and medicine. However, the method could enable hazardous or environmentally harmful materials without strong oversight. Reliance on limited metrics such as S.U.N. may favor computationally convenient but impractical candidates, while validating many outputs can be costly financially and environmentally.

AI USE STATEMENT

The text of the paper was polished for grammar and style using LLMs. We have reviewed all AI-assisted text and take responsibility for the final content of this work, including text, claims, and artifacts.

ETHICS STATEMENT

Mirage Atom Diffusion improves the diversity and quality of generated materials and may accelerate discovery in clean energy, electronics, and medicine. However, the method could enable hazardous or environmentally harmful materials without strong oversight. Reliance on limited metrics such as S.U.N. may favor computationally convenient but impractical candidates, while validating many outputs can be costly financially and environmentally.

REPRODUCIBILITY STATEMENT

Experimental details, metrics, ablations, and additional results are provided in the appendix. An anonymized archive with the raw code for all experiments is available at this link (see also Appendix G); we will release model checkpoints to further facilitate reproduction of the reported results.

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A CRYSTAL INVARIANCES

A.1 SYMMETRIES OF CRYSTAL STRUCTURE DISTRIBUTION

The space of 3D crystal structures is governed by symmetries that impose stringent constraints and play a crucial role in directing the generation process from the distribution $p(\mathcal{M})$. The model, proposed in Jiao et al. (2023) and described in Section 2.3, focuses on the following symmetries:

Permutation invariance: $\forall$ permutation $P \in S_N \implies p(L, PF, PA) = p(L, F, A)$;

$O(3)$ invariance: $\forall$ orthogonal transformation $Q \in \mathbb{R}^{3\times3} \implies p(LQ, F, A) = p(L, F, A)$;

Periodic translation invariance: $\forall$ translation $\tau \in \mathbb{R}^{1\times3} \implies p(L, w(F + \mathbf{1}\tau), A) = p(L, F, A)$;

where $w(F) = F - \lfloor F \rfloor \in [0, 1)^{N_{\text{atoms}}\times3}$ returns the fractional part of each element in F and $\mathbf{1} \in \mathbb{R}^{N_{\text{atoms}}\times1}$ is a vector of ones.

Informally, each symmetry signifies that performing a particular transformation on a crystal does not alter its likelihood under the distribution $p(\mathcal{M})$. These properties provide a strong inductive bias and can be methodically integrated into the diffusion model by design.

A.2 INVARIANT DIFFUSION MODELS

A diffusion model $p_\theta(x_0)$ is said to be invariant with respect to the symmetry group $\mathbb{G}$ if, for any transformation $g \in \mathbb{G}$, it holds that $p_\theta(g \cdot x_0) = p_\theta(x_0)$. Hoogeboom et al. (2022) proposed that invariance can be encapsulated in the diffusion model if we define:

$$\textbf{Invariant prior distribution:} \quad \forall\, g \in \mathbb{G} \implies p(x_T) = p(g \cdot x_T); \tag{3}$$

$$\textbf{Equivariant transition kernels:} \ \forall\, g \in \mathbb{G} \implies p_\theta(g \cdot x_{t-1} | g \cdot x_t) = p_\theta(x_{t-1}|x_t), \tag{4}$$

$$q(g \cdot x_t | g \cdot x_{t-1}) = q(x_t|x_{t-1}). \tag{5}$$

If conditions 3, 4 hold, then the diffusion model $p_\theta(x_0)$ is invariant with respect to the symmetry group $\mathbb{G}$ (assuming the transformation g is measure-preserving ($|\det(g)| = 1$):

$$p_\theta(g \cdot x_0) = \int p(g \cdot x_T) \prod_{t=1}^{T} p_\theta(g \cdot x_{t-1} | g \cdot x_t)\, dx_{1:T} = \int p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)\, dx_{1:T} = p_\theta(x_0),$$

whereas if conditions 4, 5 hold, then the conditional backward process is equivariant:

$$q(g \cdot x_{t-1} | g \cdot x_t, g \cdot x_0) = \frac{q(g \cdot x_t | g \cdot x_{t-1}) q(g \cdot x_{t-1} | g \cdot x_0)}{q(g \cdot x_t | g \cdot x_0)} = \\ = \frac{q(x_t|x_{t-1}) q(x_{t-1}|x_0)}{q(x_t|x_0)} = q(x_{t-1}|x_t, x_0),$$

and the training objective is invariant:

$$\mathcal{L}_g = \sum_{t=2}^{T} \gamma_t \mathbb{E}_{g\cdot x_0 \sim q(g\cdot x_0), g\cdot x_t \sim q(g\cdot x_t | g\cdot x_0)} \mathrm{KL}\left[\, q(g \cdot x_{t-1} | g \cdot x_t, g \cdot x_0) \;||\; p_\theta(g \cdot x_{t-1} | g \cdot x_t) \,\right] = \\ = \sum_{t=2}^{T} \gamma_t \mathbb{E}_{x_0 \sim q(x_0), x_t \sim q(x_t|x_0)} \mathrm{KL}\left[\, q(x_{t-1}|x_t, x_0) \;||\; p_\theta(x_{t-1}|x_t) \,\right] = \mathcal{L}.$$

The same remains true for score-matching objective if in addition to the condition 5 the following conditions are also satisfied for $\forall x, y$ – from tangent space: 6 – equivariance of the score-estimator $s_\theta(x_t, t)$, 7 – distributivity of the transformations g from the group $\mathbb{G}$, 8 – invariance of l_2-norm:

$$s_\theta(g \cdot x_t, t) = g \cdot s_\theta(x_t, t), \tag{6}$$

$$g \cdot x + g \cdot y = g \cdot (x + y), \tag{7}$$

$$||x||_2^2 = ||g \cdot x||_2^2. \tag{8}$$

Then the score-matching objective is invariant with respect to the symmetry group $\mathbb{G}$:

$$\begin{aligned}\mathcal{L}_g &= \mathbb{E}_{g\cdot x_0\sim q(g\cdot x_0),t\sim\mathcal{U}(1,T),g\cdot x_t\sim q(g\cdot x_t|g\cdot x_0)}||\nabla_{g\cdot x_t}\log q(g\cdot x_t|g\cdot x_0) - s_\theta(g\cdot x_t,t)||_2^2 = \\ &= \mathbb{E}_{x_0\sim q(x_0),t\sim\mathcal{U}(1,T),x_t\sim q(x_t|x_0)}||g\cdot\nabla_{x_t}\log q(x_t|x_0) - g\cdot s_\theta(x_t,t)||_2^2 = \\ &= \mathbb{E}_{x_0\sim q(x_0),t\sim\mathcal{U}(1,T),x_t\sim q(x_t|x_0)}||g\cdot(\nabla_{x_t}\log q(x_t|x_0) - s_\theta(x_t,t))||_2^2 = \\ &= \mathbb{E}_{x_0\sim q(x_0),t\sim\mathcal{U}(1,T),x_t\sim q(x_t|x_0)}||\nabla_{x_t}\log q(x_t|x_0) - s_\theta(x_t,t)||_2^2 = \mathcal{L}.\end{aligned}$$

The definition of the diffusion model in terms of the score function allows for the formulation of various backward transition kernels, denoted as K_θ:

$$x_{t-1} = K_\theta(x_t).$$

These kernels incorporate the score estimator s_θ in a specific manner and can be either deterministic, or stochastic. Equivariance with respect to the symmetry group $\mathbb{G}$, in the context of transition kernels K, implies the following condition in the deterministic case:

$$\forall g\in\mathbb{G},\quad K(g\cdot x) = g\cdot K(x). \tag{9}$$

In the stochastic case, this equality is sufficient. However, the necessary and sufficient condition requires equality solely in terms of probability density functions.

A.2.1 Invariances

Jiao et al. (2023) proposed that symmetric properties outlined in Section A.1 can be encapsulated in the joint diffusion model described in Section 2.3 via specific neural network parameterization.

Permutation invariance affects the components F and A. The prior distributions for these components are defined element-wise, and the corresponding transition kernels remain equivariant as long as the neural network is equivariant. It is achieved using a graph neural network (GNN) architecture that alternates between message-passing and atom-wise processing layers. The message-passing layer operates on atom pairs selected based on rules that are independent of their position in the sequence, i.e., distance cutoff between atoms. As a result, reordering of the input sequence of atoms results in the same reordering of the output sequence of predictions, ensuring permutation equivariance.

$O(3)$ invariance affects only the L component of the crystal because the F component defines coordinates within the unit cell and does not contain any information about the orientation of the unit cell in space. The prior distribution in DDPM is already invariant. In order to define an equivariant transition kernel we need to parametrize its mean in the following way:

$$\mu_\theta(\mathcal{M}_t,t) = \mu_\theta(L_t,F_t,A_t,t) = \text{NN}_\theta(L_tL_t^T,F_t,A_t,t)L_t,$$

where $\text{NN}_\theta : \mathcal{M}_t,t\to\mathbb{R}^{3\times3}$ – neural network with a linear layer on the top. Then, the following transition kernel in DDPM:

$$p_\theta\left(L_{t-1}|\mathcal{M}_t\right) = p_\theta\left(L_{t-1}|L_t,F_t,A_t\right) = \mathcal{N}\left(L_{t-1}|\mu_\theta\left(L_t,F_t,A_t,t\right),\sigma_t^2I\right),$$

is $O(3)$ equivariant:

$$\begin{aligned}p_\theta\left(L_{t-1}Q|L_tQ,F_t,A_t\right) &= \mathcal{N}\left(L_{t-1}Q|\mu_\theta\left(L_tQ,F_t,A_t,t\right),\sigma_t^2I\right) = \\ &= \mathcal{N}\left(L_{t-1}Q|\text{NN}_\theta\left(L_tQQ^TL_t^T,F_t,A_t,t\right)L_tQ,\sigma_t^2I\right) = \\ &= \mathcal{N}\left(L_{t-1}Q|\text{NN}_\theta\left(L_tL_t^T,F_t,A_t,t\right)L_tQ,\sigma_t^2I\right) = \\ &= \mathcal{N}\left(L_{t-1}Q|\mu_\theta(L_t,F_t,A_t,t)Q,\sigma_t^2I\right) = \\ &= \mathcal{N}\left(L_{t-1}|\mu_\theta(L_t,F_t,A_t,t),\sigma_t^2I\right) = \\ &= p_\theta\left(L_{t-1}|L_t,F_t,A_t\right).\end{aligned}$$

Periodic translation invariance affects only the F component. The prior distribution in Wrapped Normal diffusion is already invariant. To ensure that the transition kernel is equivariant, we parameterize the score estimator s_θ in an invariant form:

$$s_\theta(\mathcal{M}_t, t) = s_\theta(L_t, F_t, A_t, t) = s_\theta\Big(L_t, \text{PairwiseDist}(F_t), A_t, t\Big),$$
$$\text{PairwiseDist}(F_t) = \left\{\psi_{FT}(f_j - f_i) \;\middle|\; i, j = \overline{1, N_{\text{atoms}}}, i \neq j\right\},$$

where f_i – fractional coordinates of the atom i from the F_t, $\psi_{FT} : (-1, 1)^3 \to [-1, 1]^{3\times K}$ – the Fourier Transformation of the relative fractional coordinate $f_i - f_j$, and PairwiseDist : $[0, 1]^{N_{\text{atoms}}\times 3} \to [-1, 1]^{N_{\text{atoms}}\times N_{\text{atoms}}\times K}$ – yields coordinates representation which is invariant to periodic translations:

$$\text{PairwiseDist}\left(w\left(F_t + \mathbf{1}\tau\right)\right) = \text{PairwiseDist}(F_t).$$

This follows from the fact that pairwise atomic distances remain unchanged when the entire system of atoms is translated. Further, if we use the following form of the stochastic backward transition kernel K_θ:

$$F_{t-1} = K_\theta(\mathcal{M}_t) = K_\theta(L_t, F_t, A_t) = w\left(F_t + b_t s_\theta(L_t, F_t, A_t, t) + c_t\epsilon\right), \quad \epsilon \sim \mathcal{N}(0, 1),$$

where b_t, c_t are scalar coefficients, then K_θ is periodic translation equivariant (sufficient condition 9):

$$\begin{aligned} K_\theta\left(L_t, w\left(F_t + \mathbf{1}\tau\right), A_t\right) &= w\left(w\left(F_t + \mathbf{1}\tau\right) + b_t s_\theta(L_t, w\left(F_t + \mathbf{1}\tau\right), A_t, t) + c_t\epsilon\right) = \\ &= w\left(w\left(F_t + \mathbf{1}\tau\right) + b_t s_\theta(L_t, F_t, A_t, t) + c_t\epsilon\right) = \\ &= w\left(F_t + b_t s_\theta(L_t, F_t, A_t, t) + c_t\epsilon + \mathbf{1}\tau\right) = \\ &= w\left(w\left(F_t + b_t s_\theta(L_t, F_t, A_t, t) + c_t\epsilon\right) + \mathbf{1}\tau\right) = \\ &= w\left(K_\theta(L_t, F_t, A_t) + \mathbf{1}\tau\right). \end{aligned}$$

B Ablation

As discussed in Section 4, several critical steps were undertaken in developing the final version of the MiAD.

B.1 Number of mirage atoms

The definition of mirage infusion necessitates setting the hyperparameter N_m, which specifies that crystals are supplemented with mirage atoms until the total number of atoms reaches N_m. Increasing this hyperparameter results in a greater number of possible atom variants from which the model can select during crystal construction. Simultaneously, it increases the number of atoms the model must eliminate during the generation process. The neural network architecture proposed by Jiao et al.

Table 4: **Ablation study on the number of mirage atoms in MiAD** We perform a comparison of various values for N_m within MiAD: $20, 25, 30, 35$. This hyperparameter specifies that crystals are supplemented with mirage atoms until the total number of atoms reaches N_m. The models are compared using S.U.N. for 10 000 sampled crystals, where stability is estimated via (left) eq-V2 and (right) CHGNet.

Model	eq-V2 ($E^\text{hull} < 0.0$)			CHGNet ($E^\text{hull} < 0.0$)		
	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)
DiffCSP	3.8	66.6	2.5	11.3	78.8	8.9
MiAD						
$N_\text{m} = 20$	8.7	60.9	5.3	17.4	69.0	12.0
$\boldsymbol{N_\text{m} = 25}$	9.7	56.7	**5.5**	19.8	65.2	**12.9**
$N_\text{m} = 30$	8.3	56.6	4.7	16.6	68.1	11.3
$N_\text{m} = 35$	8.2	56.1	4.6	17.9	65.9	11.8

Table 5: **Ablation study of loss scaling for atom types in MiAD** We perform a comparison of the coefficients $0.5, 1.0, 2.0$ applied to the loss function for atom types in MiAD, while maintaining constant scales for the losses associated with lattice and fractional coordinates. We quantify the prioritization of the loss components corresponding to $(L-F-A)$ at the end of the training procedure as a percentage of the total loss. The prioritization for these coefficients are as follows: $\mathcal{L}_A \times 0.5$: $(40-50-10)$, $\mathcal{L}_A \times 1.0$: $(36-46-18)$, $\mathcal{L}_A \times 2.0$: $(31-39-30)$. The models are compared using S.U.N. for $10\,000$ sampled crystals, where stability is estimated via (left) eq-V2 and (right) CHGNet.

Model	eq-V2 ($E^{\text{hull}} < 0.0$)			CHGNet ($E^{\text{hull}} < 0.0$)		
	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)
DiffCSP	3.8	66.6	2.5	11.3	78.8	8.9
MiAD						
$\mathcal{L}_A \times 0.5$	8.2	57.3	4.7	17.9	68.7	12.3
$\boldsymbol{\mathcal{L}_A \times 1.0}$	9.7	56.7	**5.5**	19.8	65.2	**12.9**
$\mathcal{L}_A \times 2.0$	8.9	56.2	5.0	19.0	62.6	11.9

(2023) has a limit on the number of atoms that can interact efficiently. Beyond a certain number, the neural network loses the capacity to manage them effectively. We evaluate several variants of N_{m} in Table 4 using S.U.N. computed via MLIPs (see Appendix D), and select the optimal variant for all subsequent experiments. These results demonstrate that the proposed approach continues to be effective for values of N_{m} quite far from the optimal one, indicating that the procedure is relatively insensitive to the choice of its single hyperparameter.

B.2 Loss component prioritization

The application of mirage infusion alters the loss components associated with diffusion in fractional coordinates and atom types. This, in turn, affects gradient scales and the prioritization of the tasks the neural network must solve concurrently: 1) lattice prediction, 2) fractional coordinates prediction, and 3) atom types prediction. We found that the balance among these tasks – especially the influence of the loss component associated with atom types $\mathcal{L}_A$ (see Section 2.3.1) – can substantially affect model quality. Therefore, to isolate the effect of mirage infusion, we check this confounding factor.

We quantify the prioritization of the loss components corresponding to $(L-F-A)$ at the end of training as their percentages of the total loss. Applying mirage infusion with $N_{\text{m}} = 25$ halves the atom-type loss $\mathcal{L}_A$ and yields a balance of $(36-46-18)$ among MiAD components, whereas the balance in the original DiffCSP is $(31-39-30)$. Then, in Table 5, we compare MiAD models in which $\mathcal{L}_A$ is further increased or decreased by a factor of two; both adjustments degrade performance. Consequently, in all other experiments in the paper, we keep the balance $(36-46-18)$ between loss components without reweighting.

Overall, we consider it essential to illustrate the effects of loss reweighting in joint diffusion/flow-based models.

B.3 Definitions of mirage infusion

As discussed in Section 3, Schneuing et al. (2025) introduced a related concept involving the augmentation of original molecular structures with hypothetical (non-existent) components for structure-based drug design. In this approach, the coordinates of mirage atoms are initialized at the geometric center of mass of the real atoms, and no masking is applied to the mirage atoms. Table 6 demonstrates that this formulation (MiAD (Center + NonMasked)) fails to work for de novo crystal generation and decreases the performance of the original DiffCSP.

Table 6: **Ablation study of possible definitions of the mirage infusion** We perform a comparison of the definitions of MiAD in terms of (1) the initialization of fractional coordinates of mirage atoms in crystals: sampling from the uniform distribution or positioning at the geometric center of mass of the real atoms, (2) the masking of mirage atoms in the loss for fractional coordinates. The models are compared using S.U.N. for 10 000 sampled crystals, where stability is estimated via (left) eq-V2 and (right) CHGNet.

Model	eq-V2 ($E^{\text{hull}} < 0.0$)			CHGNet ($E^{\text{hull}} < 0.0$)		
	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)
DiffCSP	3.8	66.6	2.5	11.3	78.8	8.9
MiAD						
Unif + Mask	9.7	56.7	**5.5**	19.8	65.2	**12.9**
Center + Mask	0.5	80.0	0.4	5.8	89.7	5.2
Unif + NonMask	7.7	49.4	3.8	16.6	62.0	10.3
Center + NonMask	2.6	50.0	1.3	9.9	81.8	8.1

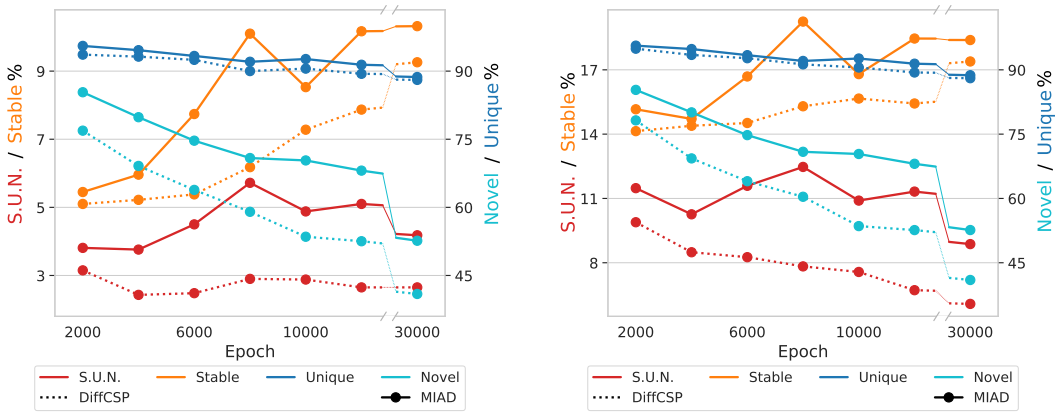

Figure 3: Comparison of MiAD (DiffCSP with mirage infusion) in its final version and DiffCSP in terms of stability, uniqueness, novelty, and S.U.N. Stability is estimated via (left) eq-V2 and (right) CHGNet. MiAD outperforms DiffCSP across all metrics, especially in terms of stability rate and S.U.N., achieving the highest quality after 8000 epochs.

B.4 Final impact of mirage infusion

Figure 3 illustrates the comparison between the final version of MiAD and the original DiffCSP. In this analysis, we employed the optimal variant of $N_{\text{m}} = 25$ as identified in Table 4. The incorporation of mirage infusion notably enhances both stability and novelty; however, it also extends the time necessary to reach peak performance.

C Related work

The field of deep generative modeling in material science has been rapidly growing in recent years. State-of-the-art approaches use a multi-step procedure for generating crystals. In this review, we organize the works by their treatment of the number of atoms during this generation process.

Models with a constant number of atoms In these models, the number of atoms is directly sampled from the prior distribution; their types and coordinates are gradually refined during the generation process along with the lattice. DiffCSP (Jiao et al., 2023) is the first pure diffusion model for crystal generation, our work directly extends their approach. Most parts of this model are described in Section 2; briefly, it is a joint diffusion model that operates with the crystal space

represented as a triplet of lattice, fractional coordinates, and atom types. The following models fall within the same paradigm: MatterGen (Zeni et al., 2025), FlowMM (Miller et al., 2024), CrysBFN (Wu et al., 2025), TGDMat (DAS et al., 2025), CrystalFlow (Luo et al., 2025). DiffCSP++ (Jiao et al., 2024) is a development of DiffCSP that constrains the diffusion process so that the crystal has predefined Wyckoff symmetries, for de novo generation they are sampled from the training dataset. ADiT (Joshi et al., 2025), uses a Transformer instead of a GNN as the denoising model.

Models with two stages In these models, the first stage is used to generate an intermediate crystal representation that includes the number of atoms, from which the structure is reconstructed during the second stage, where the number of atoms is fixed: CDVAE (Xie et al., 2021), FlowLLM (Sriram et al., 2024), WyFormer (Kazeev et al., 2025). All these models combine non-diffusion generative models in the first stage with diffusion-based refinement in the second stage.

Models that change the number of atoms These models change the number of atoms during the entire generation process, i.e., the number of atoms is generated jointly with all other components of the crystal.

The first subgroup consists of methods for changing the representation of 3D crystal structures, which allows them to vary the number of atoms during the generation process:

UniMat (Yang et al., 2023) introduces a representation that combines the periodic-table positions of atom types with geometric crystal information and applies a standard DDPM in this space. Atoms are assigned to cells of the periodic table, while unoccupied cells are represented through special coordinate encodings. These empty cells enable the model to generate new atoms during sampling. However, UniMat does not enforce rotation, translation, periodicity, and permutation invariances by design; instead, these invariances are learned through data augmentation. When applied to MP-20, UniMat relies on at least 900 empty positions and cannot be readily configured to operate with substantially fewer such positions.

CrystalDiT (Yi et al., 2026) pads the unit cell to a fixed size with dummy atoms, in spirit similar to mirage atoms. However, it neither studies their effect nor explains how their number is chosen, and it does not integrate them into a joint (L, F, A) diffusion model of the DiffCSP class while preserving rotation, translation, periodicity, and permutation equivariances and the existing data constraints. MiAD treats this factor as part of model construction. We ablate the number of mirage atoms, their initialization, and loss masking, and demonstrate their effect on de novo generation (Appendix B.1, B.3).

WyckoffDiff (Kazeev et al., 2025) constructs a diffusion model over discrete symmetry-based crystal descriptors. An analogue of mirage atoms appears as atoms in unconstrained Wyckoff positions, which can, in principle, be occupied by any number of atoms – although in practice there is a maximum. In WyckoffDiff, these "virtual atoms" arise from the choice of representation, not explicitly to enable variable atom counts. A key difference from MiAD is that, in WyckoffDiff, the positions where such atoms can appear during generation are highly constrained by the representation.

The second subgroup consists of autoregressive models: Uni-3DAR (Lu et al., 2025), CrystalFormer (Cao et al., 2025), CrystaLLM (Antunes et al., 2024), LLaMA-2 (Gruver et al., 2024).

The third subgroup consists of Crystal-GFN (Hernandez-Garcia et al., 2023) and SHAFT (Nguyen et al., 2026) – policies, which are trained using reward functions and operate in a space of 3D crystal representations along with their symmetry groups.

The fourth subgroup consists of models, which indirectly change the number of atoms during generation via changing Wyckoff positions site symmetry: SymmCD (Levy et al., 2025) and SymmBFN (Ruple et al., 2025). The diffusion/flow process, however, only deals with an asymmetric unit of fixed size.

The proposed categorization underscores the inherent limitations of diffusion-like methods in accommodating the insertion and removal of atoms during the generation process. This finding is particularly noteworthy, as leading approaches such as DiffCSP, FlowLLM, WyFormer, and ADiT are either partially or entirely based on the diffusion paradigm.

D S.U.N.

S.U.N. (Zeni et al., 2025) – the proportion of materials that are simultaneously *stable*, *unique* and *novel*. This is one of the most reasonable measures of a generative model's performance, as it directly quantifies the model's utility for materials discovery.

Novelty Represents the fraction of the generated materials that are not present in the training dataset. Following all the baselines, we use `StructureMatcher` from the `pymatgen` package (Ong et al., 2013) with the default parameters.

Uniqueness As the number of generated materials grows, a model starts to repeat itself. Uniqueness is the fraction of unique materials among generated, also estimated with `StructureMatcher`.

Stability To be useful, a material must actually exist under normal conditions. Ab initio prediction of experimental stability is an open research question (Tolborg et al., 2022; Sun et al., 2016) with various trade-offs between the accuracy and computational cost possible. Again, we follow state-of-the-art ML baselines (Miller et al., 2024; Kazeev et al., 2025; Zeni et al., 2025; Joshi et al., 2025) and use *energy above convex hull* E^{hull} as the stability measure. There are two important nuances.

(1) Stability condition If a material has positive E^{hull}, this indicates that the same set of atoms can be rearranged into a known different configuration with a lower potential energy. This, however, does not necessarily mean that the higher-energy material will not exist under normal conditions; for example, both graphite and diamond do. We, therefore, measure the number of both *stable* materials with $E^{\text{hull}} < 0$ eV that are highly likely to exist; and *metastable* materials with $E^{\text{hull}} < 0.1$ eV, which are likely, but not certain to exist; the choice of the threshold follows Joshi et al. (2025).

(2) Energy computation method Density Functional Theory (DFT) (Kohn & Sham, 1965) is the ab initio method that has been used to obtain the energy values and structures in Materials Project (Jain et al., 2013), used both as training data and convex hull. We use DFT to support the main claims of our paper, to evaluate the performance of MiAD, and compare it to the baselines in Table 1; the computation details are described in Appendix F. Due to the large computational cost of DFT, not all baseline works use it for stability evaluation, some opt for Machine Learning Interatomic Potentials (MLIPs). MLIPs are a rapidly advancing research area, useful for stability estimation (Riebesell et al., 2023), but still fall short of DFT accuracy (Deng et al., 2025), as evident by S.U.N. values difference for the same models in Tables 1 and 2. We use two MLIP models, CHGNet (Deng et al., 2023) and eq-V2 (Barroso-Luque et al., 2024), for ablation studies and for a supplementary comparison with baseline methods for which DFT data are not available. In the cases of DFT or CHGNet, we first prerelax crystals via CHGNet for 1500 steps, while in the cases of eq-V2, we prerelax via eq-V2 for 100 steps.

E Additional metrics

While S.U.N. remains the principal criterion for evaluating modern generative models in de novo crystal generation Miller et al. (2024); Sriram et al. (2024); Joshi et al. (2025), it is instructive to consider additional metrics that are being used in the literature. These include Structure Validity, Compositional Validity, Coverage (COV-R, COV-P), and distributional distances such as the Wasserstein distance of scalar material properties (e.g., density, number of elements), proposed in Xie et al. (2021). Such metrics provide complementary perspectives on model performance, quantifying local consistency of atomic structures or alignment with empirical property distributions.

However, these measures exhibit important limitations. Particularly, Validity and Coverage are nearly saturated for modern models, as shown in Table 7, with reported differences between approaches often below 1%. More critically, they fail to penalize overfitting. For example, if the MP-20 training set is itself evaluated as a "generative model", it achieves near-optimal values across Validity and Coverage, underscoring that such metrics can be artificially inflated just by replication of training data. Consequently, a model that prioritizes memorization over discovery may appear competitive according to these statistics, despite offering little value for materials discovery.

An illustrative case can be drawn by comparing MiAD with FlowLLM. FlowLLM reports a higher Compositional Validity (89.05% vs. 84.21%), yet its Uniqueness & Novelty (U&N) rate shown

Table 7: Evaluation of MiAD on Perov-5, Carbon-24, and MP-20 datasets compared with baseline models. All results follow the same mirage infusion configuration as for MP-20.

		Validity (%)↑		Coverage (%)↑		Property (%)↓	
Data	Method	Struc.	Comp.	COV-R	COV-P	d_ρ	d_{elem}
Perov-5	DiffCSP	100.00	98.85	99.74	98.27	0.111	0.013
	CrysBFN	100.00	98.86	99.52	98.63	0.073	0.010
	TGDMat	100.00	98.63	99.83	99.52	0.050	0.009
	MiAD	94.82	97.91	98.07	92.82	0.089	0.075
Carbon-24	DiffCSP	100.00	NA	99.90	97.27	0.081	NA
	CrysBFN	100.00	NA	99.90	99.12	0.061	NA
	TGDMat	100.00	NA	99.99	92.43	0.043	NA
	Uni-3DAR	99.99	NA	100.00	98.16	0.066	NA
	MiAD	99.85	NA	99.51	99.46	0.061	NA
MP-20	DiffCSP	100.00	83.25	99.71	99.76	0.350	0.340
	UniMat	97.20	89.40	99.80	99.70	0.088	0.056
	FlowMM	96.85	83.19	99.49	99.58	0.239	0.083
	FlowLLM	99.81	89.05	99.06	99.68	0.660	0.090
	SymmCD	90.34	85.81	99.58	97.76	0.230	0.400
	WyFormer+DiffCSP++	99.80	81.40	99.51	95.81	0.360	0.079
	SymmBFN	94.27	83.93	99.73	99.00	0.083	0.095
	CrysBFN	100.00	87.51	99.09	99.79	0.207	0.163
	TGDMat	100.00	92.97	99.89	99.95	0.338	0.289
	Uni-3DAR	99.89	90.31	99.62	99.83	0.477	0.069
	MiAD	99.25	84.21	99.35	99.80	0.233	0.027
	MP-20 Train	100.00	90.65	99.81	99.79	0.133	0.025

in Table 1 is markedly lower (33.8% vs. 65.2%). The discrepancy arises because FlowLLM predominantly reproduces training set compositions, which maximizes apparent validity while suppressing novelty. In contrast, MiAD sacrifices a small degree of compositional accuracy but generates a significantly larger proportion of genuinely new materials, which is the central objective of de novo generation.

To further validate the proposed MiAD approach, we conducted the experiments with small-scale datasets, Perov-5 and Carbon-24. For both of them, we employed the same mirage infusion configuration as for MP-20, specifically $N_{\text{m}} = N + 5$, where N is the maximum number of atoms in crystals in each respective dataset (i.e., $N_{\text{m}} = 10$ for Perov-5 and $N_{\text{m}} = 29$ for Carbon-24). All other hyperparameters (batch size, number of epochs, and neural network architecture) were adopted directly from DiffCSP.

A comparison of models trained on the Perov-5 and Carbon-24 datasets using the S.U.N. metric is not meaningful because both datasets contain materials that are thermodynamically unstable under standard conditions Xie et al. (2021). Consequently, recent studies Zeni et al. (2025); Miller et al. (2024); Sriram et al. (2024); Joshi et al. (2025); Kazeev et al. (2025) have discontinued the use of these two datasets for benchmarking de novo generation. Currently, there are no well-established methods for fair comparison on these datasets that penalize overfitting. Therefore, Validity, Coverage, and Property could be used only to validate the model's ability to generate coherent structures, while ignoring overfitting. In this light, Table 7 shows that MiAD is competitive with the prior baselines.

This analysis highlights why S.U.N. remains the most informative single metric. Unlike isolated measures, S.U.N. directly evaluates the trade-off between replicating known structures and discovering stable, previously unobserved crystals, thereby capturing the utility of generative models in the materials discovery pipeline. While auxiliary metrics may still be valuable for diagnostic purposes, they should be interpreted with caution, as they may obscure or even contradict the overarching goal of novelty-driven generation.

F DFT COMPUTATION DETAILS

We use DFT settings from Materials Project `https://docs.materialsproject.org/methodology/materials-methodology/calculation-details/gga+u-calculations/parameters-and-convergence` for structure relaxation and energy computation. In particular, we do GGA and GGA+U calculations with `atomate2.vasp.flows.mp.MPGGADoubleRelaxStaticMaker` (Ganose et al., 2025), which in turn relies on `pymatgen.io.vasp.sets.MPRelaxSet` and `pymatgen.io.vasp.sets.MPStaticSet` (Ong et al., 2013). Computations themselves were done with VASP (Kresse & Furthmüller, 1996) version 5.4.4. The raw total energies computed by DFT were corrected with `MaterialsProject2020Compatibility` before putting into the `PhaseDiagram` to obtain the DFT E^{hull}. We used the MP convex hull `2023-02-07-ppd-mp.pkl.gz` distributed by `matbench-discovery` (Riebesell et al., 2023) as the reference hull.

G EXPERIMENTAL DETAILS

G.1 CODE

An anonymized zip archive containing the raw code for all the experiments is accessible for download through this link.

G.2 DATASET

All experiments were conducted using the MP-20 dataset (Jain et al., 2013), which comprises 45,231 stable inorganic materials selected from Material Projects (Jain et al., 2013). We employed the same train-validation-test split of 60-20-20 as used in the study by Xie et al. (2021).

G.3 NEURAL NETWORK ARCHITECTURE

The models utilized the CSPNet neural network architecture proposed by Jiao et al. (2023), with the following hyperparameters: ”hidden_dim” : 512, ”num_layers” : 6, ”num_freqs” : 128, ”latent_dim” : 256, ”max_atoms” : 100, ”act_fn” : ”silu”, ”dis_emb” : ”sin”, ”edge_style” : ”fc”, ”max_neighbors” : 20, ”cutoff” : 7.0, ”ln” : True, ”ip” : True. The application of mirage infusion, which necessitates the use of an additional atom type 0 in the D3PM diffusion module corresponding to atom types (refer to Sections 2.3.1 and 3), does not increase the number of neural network parameters. This is because the configuration proposed by Jiao et al. (2023) already includes several free atom types that can be utilized in the proposed model.

G.4 OPTIMIZATION

Jiao et al. (2023) advocated using a batch size of 256 with the Adam optimizer (Kingma, 2014), an initial learning rate of 10^{-3}, and a scheduler that reduces the learning rate to 10^{-4} when the validation loss ceases to decrease. However, we observed that this scheduler does not affect the S.U.N. values of the original DiffCSP, and therefore omitted it from our experiments as an unnecessary complication. Consequently, throughout our experiments with the DiffCSP and MiAD models (Figures 2 and 3), we adopted a simpler optimization strategy than that proposed by Jiao et al. (2023). We found that 1000 epochs were sufficient to train the original DiffCSP model, but inadequate for a model after the application of mirage infusion. For the best-performing version of mirage infusion, maximum performance (S.U.N. computed via eq-V2) was achieved after 8000 epochs (Figure 3). This increase in training budget is intuitively expected given the greater task difficulty in MiAD relative to DiffCSP, due to:

- more atoms per crystal, leading to a greater number of denoising sub-tasks;
- an additional atom type, resulting in more prediction variants;
- varying positions of mirage atoms, which effectively augment the dataset.

Table 8: **Scaling mirage infusion to MPTS-52** MiAD is trained with $N_{\text{m}} = 57$. MiAD-WRNA is trained with $N_{\text{m}} = N_{\text{atoms}} + k$, where $k \sim \mathcal{U}[0, 10]$ (+5 mirage atoms in average). The models are compared using S.U.N. for 10 000 sampled crystals, where stability is estimated via (left) eq-V2 and (right) CHGNet.

Model	eq-V2 ($E^{\text{hull}} < 0.0$)			CHGNet ($E^{\text{hull}} < 0.0$)		
	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)
DiffCSP	4.3	37.2	1.6	11.8	69.9	8.2
MiAD	5.7	55.6	**3.2**	13.0	76.2	**9.9**
MiAD-WRNA	5.6	44.1	2.5	13.0	70.9	9.2

G.5 Computational costs

The proposed mirage infusion technique (see Section 3) substantially increases the average number of atoms with which the neural network interacts during the training and sampling procedures, leading to increased time and memory costs. After applying the mirage infusion technique in its optimal configuration ($N_{\text{m}} = 25$, which corresponds to approximately a $\times 2.7$ increase in the average number of atoms in the crystals), we observe the following approximate increases in execution time: training step $\times 4.3$, sampling step $\times 3.8$; and the following approximate increases in memory consumption: training step $\times 4.4$, sampling step $\times 4.6$. These estimates were obtained on a single GPU NVIDIA Tesla V100 32 GB with 4 CPU cores Intel Xeon Gold 6152 (2.1–3.7 GHz). In our experiments, MiAD ($N_{\text{m}} = 25$) required 4 days for the training procedure (8000 epochs) and 2 hours for the sampling procedure (10 000 crystals) on 2 GPUs NVIDIA Tesla A100 80 GB with 8 CPU cores AMD EPYC 7702 2-3.35 GHz. The training and sampling procedures can also be conducted on a single GPU, though this will incur increased time costs.

H Scalability on crystals with larger number of atoms

Mirage infusion enables a joint diffusion model operating on the (L, F, A) crystal representation to change the number of atoms in a crystal during generation. To assess how this procedure scales when the admissible range of atom counts is wider, we conduct experiments on MPTS-52 – a more challenging extension of MP-20 (Jain et al., 2013), comprising 40,476 structures with up to 52 atoms per cell, ordered by earliest publication year in the literature.

There are several challenges in conducting comparisons on MPTS-52. To our knowledge, prior works have not reported wide comparisons of S.U.N. metrics for different generative models on MPTS-52. Metrics such as Structure Validity, Compositional Validity, Coverage (COV-R, COV-P), and distributional distances (e.g., the Wasserstein distance of scalar material properties such as density or number of elements) proposed in (Xie et al., 2021) have significant limitations, which we discuss in Appendix E. It is important to consider the DiffCSP backbone architecture, which operates most effectively with crystals containing fewer than 20 atoms. Applying DiffCSP to MPTS-52 places the model in a regime where performance degrades due to the larger number of atoms. Applying mirage infusion further increases the number of atoms; thus, when we use the same network architecture, that challenge is amplified.

We trained the original DiffCSP and MiAD on MPTS-52 for 6k epochs (six times the number of epochs used in the original DiffCSP for MPTS-52) and selected the best checkpoints by S.U.N. We use the same neural network as in experiments on MP-20. We did not tune MiAD for MPTS-52, but instead used the configuration identified as optimal on MP-20:

MP-20: $N_{\text{m}} = \text{maximum_number_of_atoms_in_mp20} + 5 = 20 + 5 = 25$

MPTS-52: $N_{\text{m}} = \text{maximum_number_of_atoms_in_mpts52} + 5 = 52 + 5 = 57$

The results are presented in Table 8. Here, we observe consistent improvements with mirage infusion using the same configuration (without finding optimal hyperparameters for dataset). Computational overhead: 1 epoch of DiffCSP training on MPTS-52: 35 sec, while 1 epoch of MiAD ($N_{\text{m}} = 57$)

Table 9: **Comparison of MiAD and MatterGen trained on Alex-MP20** We report stability and S.U.N. estimated eq-V2 for 10 000 sampled crystals. For clarity in evaluating the model's quality, we also report the Unique&Novel rate among stable crystals.

Model	eq-V2 ($E^{\text{hull}} < 0.0$)		
	Stable (%)	Unique&Novel (%)	S.U.N. ↑ (%)
MatterGen	5.2	39.4	2.1
MiAD	7.1	35.3	**2.5**

training on MPTS-52: 79 sec (≈ 2.26x compared to DiffCSP). The overhead is smaller than in MP-20 (see Appendix G) because the network is already near its upper limit of effective atomic interactions (20 atoms); further increases in atom count then lead to approximately linear, not quadratic, scaling.

Applying mirage infusion to datasets with a broad range of atom counts is a plausible use case in practical applications. For such datasets, we can vary the number of mirage atoms added per structure while keeping the rest of the procedure unchanged. We demonstrate this variant on MPTS-52. Specifically, we set N_{m} per crystal to $N_{\text{atoms}} + \text{Uniform}[0, 10]$, i.e., each crystal receives 0-10 mirage atoms (+5 on average). At generation start, we sample the number of atoms from the training-set distribution (as in the original DiffCSP), and add a sample from $\text{Uniform}[0, 10]$. The results for this variant (MiAD-WRNA: MiAD for Wide Ranges of Number of Atoms) presented in Table 8. MiAD-WRNA still provides substantial gains over DiffCSP, although it performs slightly worse than the original MiAD with fixed N_{m}. Its main advantage lies in computational cost: 1 epoch of DiffCSP training on MPTS-52: 35 sec; 1 epoch of MiAD ($N_{\text{m}} = 57$) training on MPTS-52: 79 sec (≈ 2.26x vs DiffCSP); 1 epoch of MiAD-WRNA (+5 avg) training on MPTS-52: 40 sec (≈ 1.14x vs DiffCSP). Thus, MiAD-WRNA offers a practical trade-off between computational cost and quality.

These MPTS-52 experiments, together with Table 4, support the effectiveness of mirage atoms across different strategies for incorporating them into crystals.

I Comparison on Alex-MP20

To demonstrate the scalability of MiAD, we conduct experiments on the large-scale Alex-MP20 dataset (Zeni et al., 2025) and compare its performance with that of MatterGen. We employ S.U.N., estimate stability using eq-V2, and use the same energy hull as in the previous experiments. The only difference in the evaluation protocol is that novelty is measured relative to the Alex-MP20 training set. Samples from both models are pre-relaxed for 100 steps using eq-V2. MiAD is trained for 1200 epochs with the same hyperparameters as in the MP-20 experiments. The results in Table 9 demonstrate that MiAD, without additional hyperparameter tuning, achieves state-of-the-art performance on one of the largest datasets for de novo crystal generation.

J Distribution of number of atoms

Mirage infusion incorporates the ability to insert and remove atoms during the generation process. However, we must verify that the model actually learns to use this capability. To this end, we report statistics on the number of atoms in S.U.N. crystals generated by MiAD (see Figure 4).

$p(A_{T,i}) = \text{Cat}(A_{T,i} \mid \mathbf{1}/(N_{\text{types}} + 1))$ – atom types (including the mirage type) have a uniform prior (see Section 2.3.1)), where $N_{\text{types}} = 100$ in practice. Thus, if we use mirage infusion with $N_m = 25$, then at the start of generation ($t = T$) all atoms in a crystal are real with probability ≈ 0.77, exactly one atom is mirage with probability ≈ 0.19, and so on. This implies that, at the start of generation, almost all crystals contain more than 23 real atoms. This fact, together with the statistics in Figure 4, demonstrates that MiAD

- changes the number of atoms in a crystal during generation;
- generates S.U.N. crystals with different numbers of atoms.

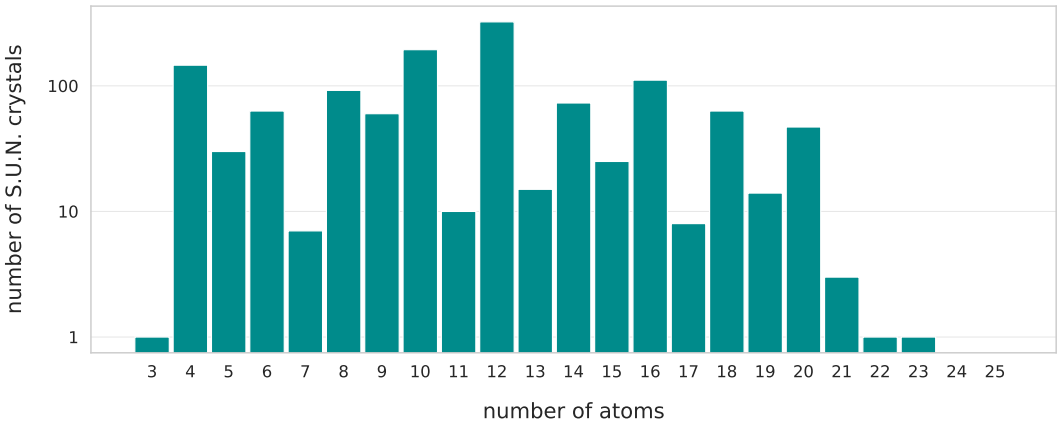

Figure 4: Number of atoms in S.U.N. crystals generated by MiAD. We consider only S.U.N. crystals among the 10 000 crystals generated by MiAD. After generation, crystals are prerelaxed via CHGNet. Stability is also estimated via CHGNet.

Crystals with $3, 7, 11, 13, 17$ atoms appear more rarely than others, because crystals with these atom counts are underrepresented in the training data.

Crystals with more than 20 atoms are automatically considered novel, because the MP-20 dataset contains only crystals with no more than 20 atoms. On the one hand, this indicates the generative model's generalizability. On the other hand, MiAD generates only 5 S.U.N. crystals with more than 20 atoms out of 10 000, which corresponds to 0.05% of the generated crystals. This means that MiAD surpasses its competitors not due to an ability to generate crystals with more than 20 atoms (which those models lack), because even if these 0.05% are excluded from the 12.9% of S.U.N. crystals, the resulting S.U.N. is approximately 12.8%, which remains higher than that of CrystalDiT (12.3%), the nearest rival in Table 2.

K SPACEGROUP DISTRIBUTION

Diversity is a key aspect of the quality of a generative model. S.U.N. addresses this aspect via U – uniqueness. However, this is not the only relevant evaluation, because crystals can differ from one another in various ways. At the same time, many existing diffusion-like models (as well as MiAD) for crystal generation cannot guarantee that the generated crystals will span different spacegroups (particularly the more complex ones, such as cubic or hexagonal). The common assumption is that a diffusion model will learn this from the training data.

To address these concerns, we compare the number of S.U.N. crystals belonging to each spacegroup among 10 000 crystals generated by different models and prerelaxed using CHGNet (see Figure 5). Based on this experiment, we can derive the following claims:

- Existing generative models for crystals do not suffer from severe mode collapse;
- MiAD, on average, generates more S.U.N. crystals than other models without exhibiting mode collapse.

From the application perspective, we argue that the particular shape of the spacegroup distribution is not one of the primary aspects of generative model quality in materials discovery. A spacegroup distribution that is closest to the train or test distribution, or that is the most uniform, does not by itself indicate clear benefits of a particular generative model for the task of inventing novel materials. At the same time, the shape of such distributions can indicate drawbacks if the generative model completely ignores crystals from a particular spacegroup. Our main point is that we should not conflate distribution-based quality criteria with S.U.N., but rather use

- S.U.N. as an averaged quality measure;

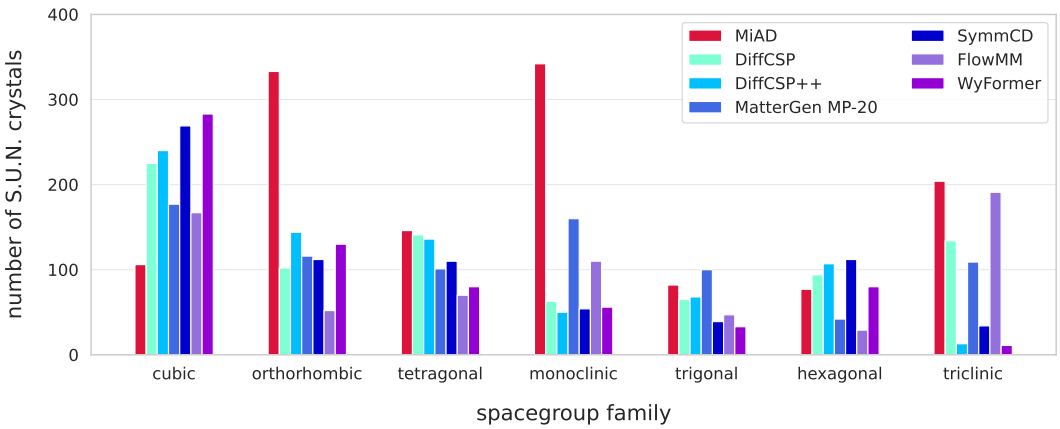

Figure 5: Comparison of models for de novo crystal generation in terms of numbers of S.U.N. crystals belonging to main spacegroup families. We categorize only S.U.N. crystals produced by generative models with a fixed budget of 10 000 generated crystals. After generation, crystals are prerelaxed via CHGNet. Stability is also estimated via CHGNet. Spacegroup families are identified via `SpacegroupAnalyzer` from the `pymatgen` package with tolerance: 0.1.

- distribution-based metrics as diagnostics to check for the absence of serious diversity issues.

Finally, we note that, after the end of diffusion generation, the resulting crystals contain mirage atoms and exhibit no symmetries, because the positions of the mirage atoms are random. This occurs because, at the training stage, our design choices – expanded domain and loss modifications – did not encourage the model to place mirage atoms at particular positions. However, after removing the mirage atoms, these crystals become symmetric. This indicates that the model continues to learn the underlying symmetries, but applies them only to the real (non-mirage) atoms rather than to all atoms.

This indicates that the model learns to construct symmetric structures using real atoms and successfully refrains from using mirage atoms to realize these symmetries.

L Qualitative analysis of mirage infusion dynamics

The proposed MiAD framework generalizes standard crystal diffusion models by introducing dynamic atom counts. This approach differs from fixed-size baselines along three primary axes: (1) the formulation of the generative task, (2) the robustness of generation trajectories, and (3) the expanded action space available during diffusion. While the first two axes are implicit, the third, the ability to dynamically add or remove atoms, enables a direct analysis of how the model manages structural evolution. In this section, we investigate the hypothesis that mirage atoms provide an ”error correction” mechanism, allowing the model to recover from unstable intermediate states.

L.1 Methodology

To isolate the impact of the mirage mechanism, we focused on ”boundary” cases in the generation trajectories where the model converts a real atom into a mirage atom (effectively removing it) during the final stages of the reverse diffusion process. We performed a comparative analysis on these samples, defined as follows:

The Counterfactual (M_t): The structure at the moment right before the last change in the denoising trajectory from a real atom to a mirage atom. In this state, the atom remains a real element, simulating a fixed-size model that cannot delete atoms, even when they are structurally disadvantageous.

The Corrected Structure ($\hat{M}_t$): The crystal structure with the same set of atoms as right after the model successfully changed the real atom to the mirage atom. To ensure that differences arise solely

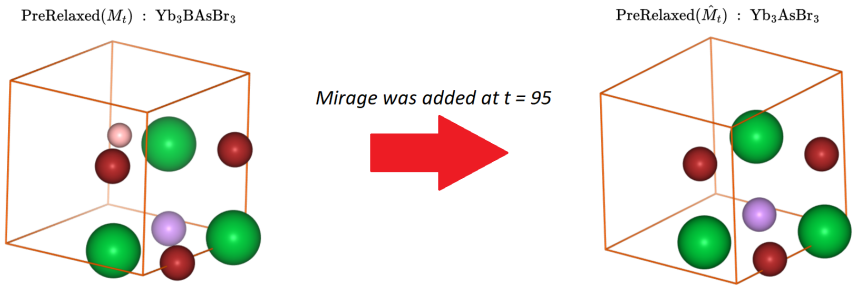

Figure 6: Comparison between the counterfactual structure M_t (left), and the corrected structure $\hat{M}_t$ (right). The corrected structure is thermodynamically stable with a higher symmetry group (monoclinic) compared to the unstable, triclinic counterfactual.

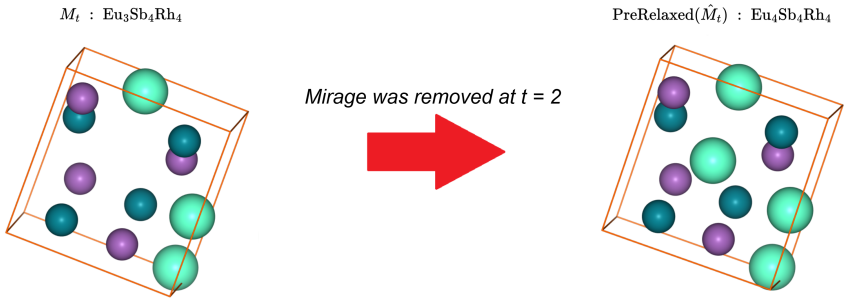

Figure 7: Comparison between the intermediate counterfactual structure M_t (left) and the corrected structure $\hat{M}_t$ (right) after a mirage atom transitions into a real Europium atom at $t = 2$. The dynamic completion of the lattice restores orthorhombic symmetry and secures thermodynamic stability.

from the composition change (and not from stochastic noise or drift), we preserve the exact lattice parameters and fractional coordinates of all remaining atoms from M_t.

Both M_t and $\hat{M}_t$ were subsequently pre-relaxed using CHGNet to evaluate their stability and symmetry properties.

L.2 Evidence of error correction

Our observations reveal that the mirage mechanism functions as a dynamic pruning tool. Out of 1000 generated crystals, we analyzed a subset of 57 that were identified as Stable, Unique, and Novel, where the transition from a real atom to a mirage occurred after 150 steps of the denoising process (out of 1000).

The removal of the superfluous atoms in these trajectories resulted in drastic improvements in thermodynamic stability:

1. The median energy above hull (E^{hull}) dropped from 0.29 eV/atom for the counterfactuals (M_t) to 0.033 eV/atom for the corrected structures ($\hat{M}_t$).
2. The median absolute deviation of the energy narrowed significantly from 0.27 to 0.12, indicating a more consistent convergence toward stable minima.

Furthermore, the structural symmetry improved substantially. Among the 57 crystals, only 14 exhibited non-trivial symmetry groups (cubic, monoclinic, orthorhombic, triclinic, or trigonal) in the uncorrected state. After the mirage infusion, this number nearly doubled to 27 crystals. This suggests that the model effectively removes atoms that break symmetry or disrupt the lattice, a capability structurally impossible for fixed-size diffusion baselines.

L.3 CASE STUDY: REAL TO MIRAGE TRANSITIONS

A concrete example illustrates this behavior: in one trajectory (see Figure 6), the model removed a Boron atom at step 95 (of 1000), shifting the composition from Yb_3BAsBr_3 (M_t) to Yb_3AsBr_3 ($\hat{M}_t$). While both structures initially possessed triclinic symmetry, the pre-relaxed crystal $\hat{M}_t$ converged to a higher-symmetry monoclinic group and achieved thermodynamic stability (negative energy above hull, -0.083 eV/atom). Conversely, the counterfactual M_t failed to find higher symmetry, remaining triclinic, and was found to be heavily unstable (0.335 eV/atom).

This confirms that the mirage atoms allow the model to alleviate mistakes made during earlier stages of generation, dynamically refining the composition to ensure realizability.

L.4 CASE STUDY: MIRAGE TO REAL TRANSITIONS

Conversely to the dynamic pruning described above, the model also utilizes the transition from a mirage to a real atom to complete missing structural components and stabilize the lattice.

To illustrate this, we examine a generative trajectory for $Eu_4Sb_4Rh_4$ (see Figure 7). At the moment right before the final Europium atom materialized from a mirage placeholder ($t = 2$), the intermediate counterfactual structure (M_t: $Eu_3Sb_4Rh_4$) was triclinic ($E^{\text{hull}} = -0.002$ eV/atom). Upon relaxation, this incomplete lattice structurally fails, yielding a highly unstable state with $E^{\text{hull}} = 0.833$ eV/atom.

However, when the model correctly transforms the mirage into the real Eu atom ($\hat{M}_t$: $Eu_4Sb_4Rh_4$), it completes the lattice. The corrected structure achieves orthorhombic symmetry ($E^{\text{hull}} = -0.118$ eV/atom before relaxation) and converges to a highly stable minimum ($E^{\text{hull}} = -0.126$ eV/atom after relaxation). This demonstrates that mirage infusion works as an explicit error-correction mechanism that allows the model to dynamically recover from brittle intermediate states.