SymADiT: Symmetry-Aware Crystal Generation with Latent Flow Matching

arXiv

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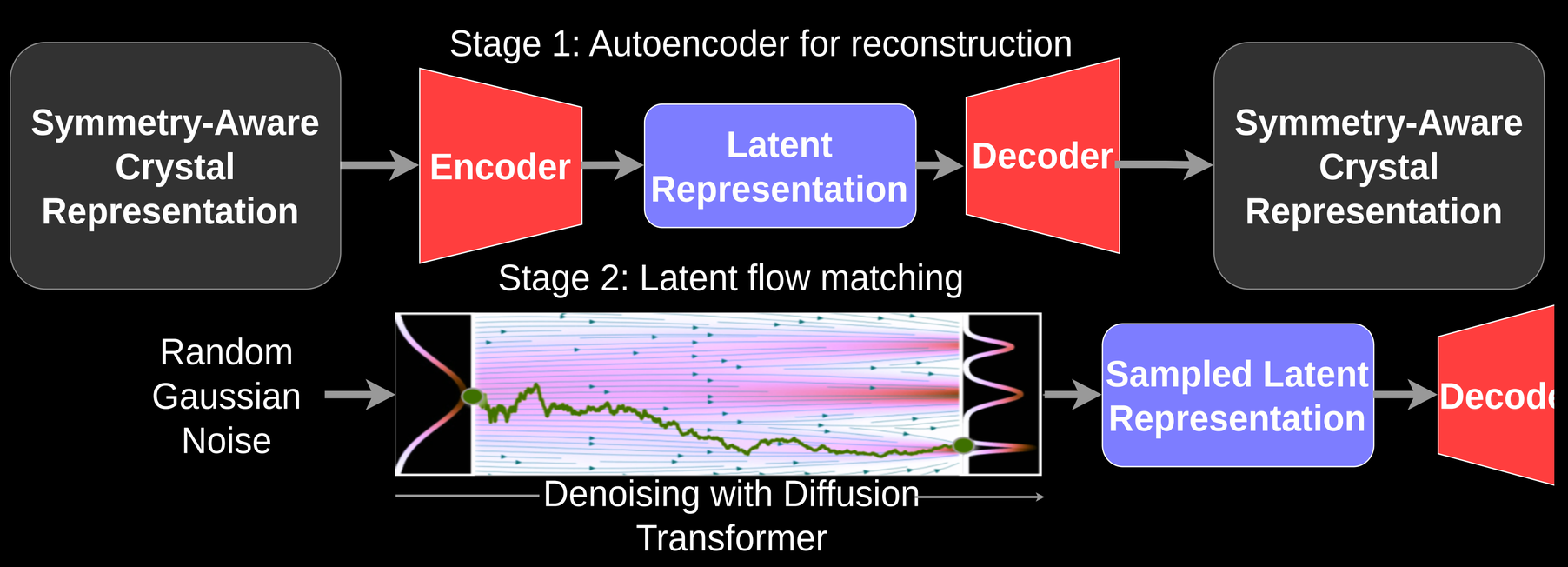
Computer Vision and Learning Systems & AI4X, Linköping University

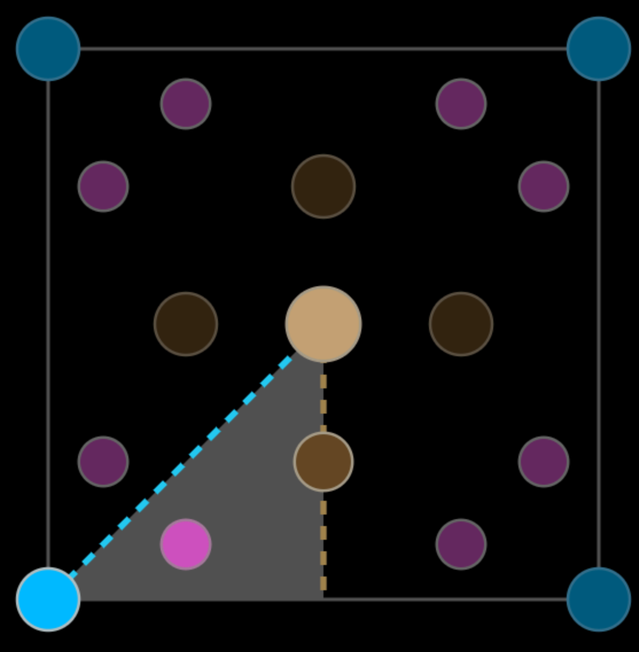
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TL;DR: SymADiT turns a symmetry-agnostic latent flow model into a symmetry-aware crystal generator using space groups and Wyckoff positions

Intro: Crystals in nature exhibit crystallographic symmetry, making symmetry a strong inductive bias for crystal generation: rather than learning symmetry implicitly from data, SymADiT encodes it explicitly via space groups and Wyckoff positions

SymADiT: Architecture and Wyckoff Representation





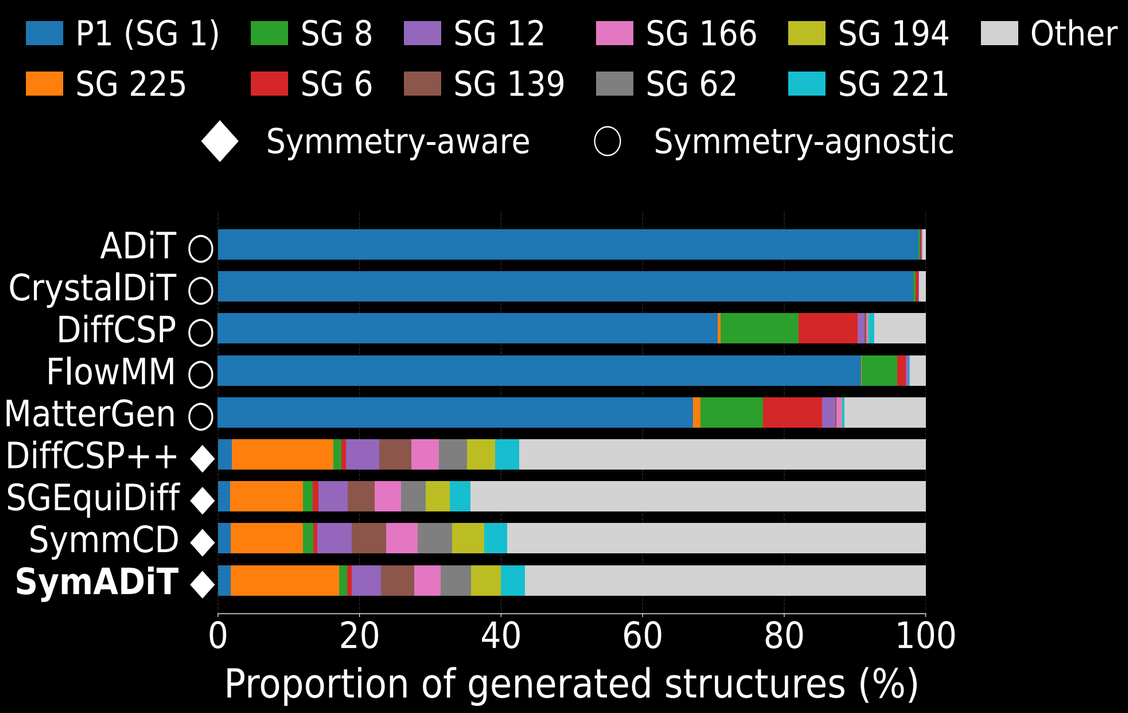
SymADiT: Two-stage latent generative model

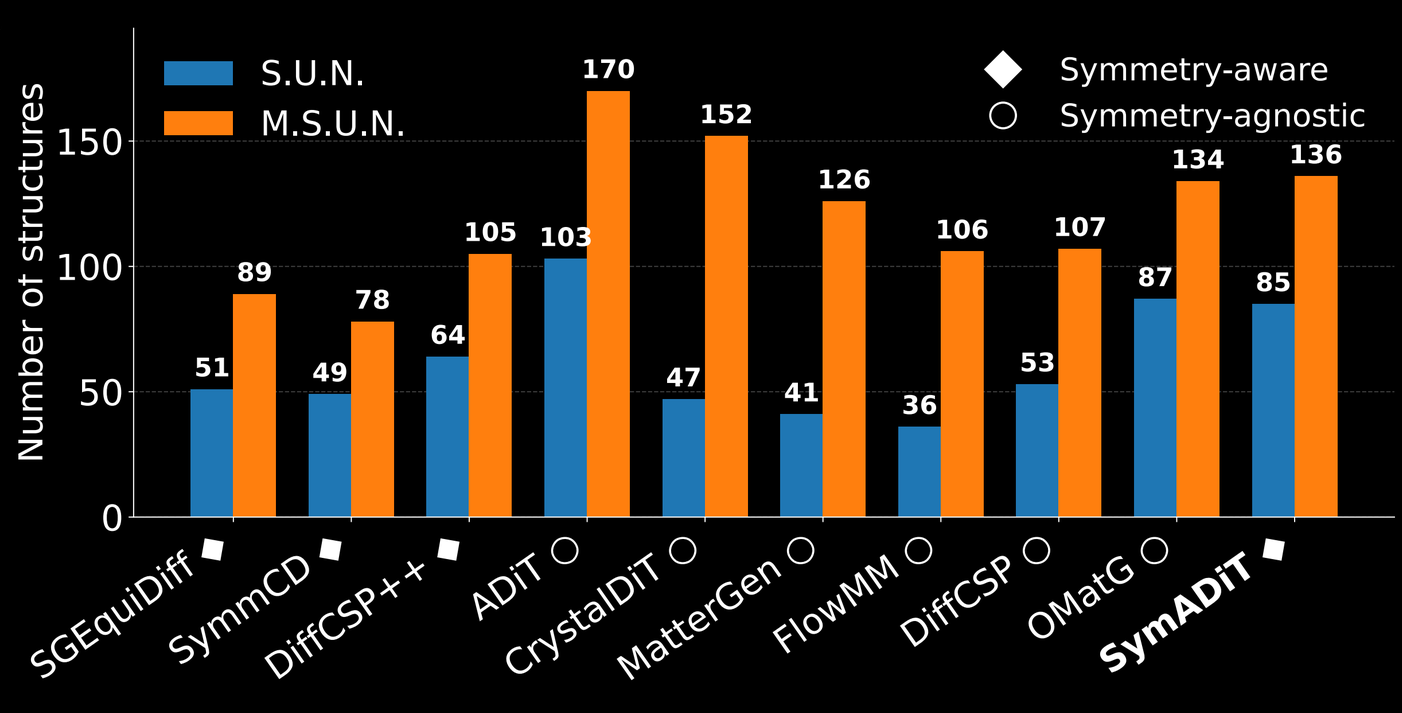
1. Symmetry-aware autoencoder with Transformer
2. Latent Flow Matching with Diffusion Transformer

Why Wyckoff positions?

- Symmetry by construction
- Avoids redundant encoding of symmetry-equivalent atoms
- Fewer tokens

Experimental Results





- Symmetry-agnostic methods struggle with capture symmetry in the data - generating mainly P1 structures
- **SymADiT** achieves the highest S.U.N. and M.S.U.N. among symmetry-aware methods
- **SymADiT** uses a simple off-the-shelf Transformer - no specialized architecture required
- **SymADiT** gives 2.40x reduction in total generation time compared with ADiT

Main Takeaways

- **Explicit crystallographic symmetry provides a strong inductive bias for crystal generation**
- **An off-the-shelf Transformer is sufficient for symmetry-aware crystal generation**