Fourier Transformers for Latent Crystallographic Diffusion and Generative Modeling

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The discovery of new crystalline materials calls for generative models that handle periodic boundary conditions, crystallographic symmetries, and physical constraints, while scaling to large and structurally diverse unit cells. We propose a reciprocal-space generative framework that represents crystals through a truncated Fourier transform of the species-resolved unit cell atomic density, rather than modeling atomic coordinates directly. This representation is periodicity-native, admits simple algebraic actions of spacegroup symmetries, and naturally supports variable atomic multiplicities during generation, addressing common major limitations of particle-based approaches such as GNN-based diffusion models [1-3]. Using only 9 Fourier basis functions per spatial dimension, our approach is able to reconstruct unit cells containing up to 208 atoms per chemical species for highly symmetric cells. We instantiate this pipeline with a transformer-based model composed of a variational autoencoder (VAE) applied on complex-valued Fourier coefficients (See fig. **1a** and **1b**), paired with a latent diffusion model that generates in the compressed latent space. We trained and benchmarked the model on a curated dataset based on the recent LeMat-BulkUnique dataset from the LeMaterial database [4], which gathers and standardize data from 3 major DFT-computed crystal databases: the Materials Project [5], Alexandria [6] and the Open Quantum Materials Database [7]. We then compared unconditional generation against re-trained coordinate-based baselines. Most notably, our model addresses one of the biggest limitations of most unconstrained state-of-the-art models for crystal generation by being able to learn and generate highly symmetric spacegroups common position patterns such as perovskite cells without any explicitly enforced symmetry processing. This opens the way for more powerful models development for crystal configuration space exploration.

References

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Figures

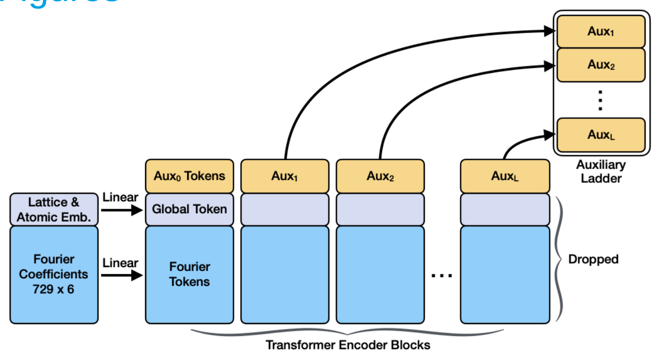

Figure 1a: Complex Fourier Transformed coefficients Encoder.

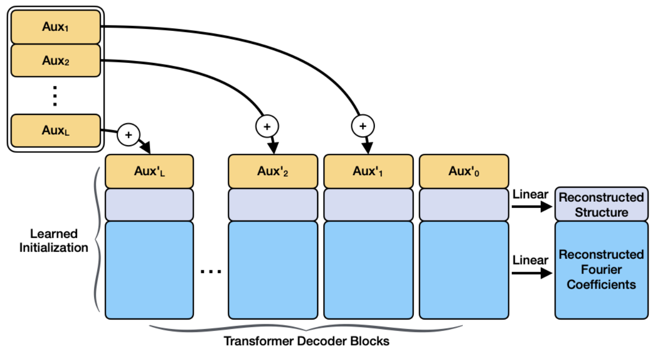

Figure 1b: Complex Fourier Transformed coefficients Decoder.