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CrystalFormer

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We introduce CrystalFormer, a transformer-based autoregressive model specifically designed for space group-controlled generation of crystalline materials. The space group symmetry significantly simplifies the crystal space, which is crucial for data and compute efficient generative modeling of crystalline materials. Leveraging the prominent discrete and sequential nature of the Wyckoff positions, CrystalFormer learns to generate crystals by directly predicting the species and locations of symmetry-inequivalent atoms in the unit cell. Our results demonstrate that CrystalFormer matches state-of-the-art performance on standard benchmarks for both validity, novelty, and stability of the generated crystalline materials. Our analysis also shows that CrystalFormer ingests sensible solid-state chemistry information from data for generative modeling. The CrystalFormer unifies symmetry-based structure search and generative pre-training in the realm of crystalline materials. The simplicity, generality, and flexibility of CrystalFormer position it as a promising architecture to be the foundational model of the entire crystalline materials space, heralding a new era in materials modeling and discovery.

Primary author: WANG, Lei (Institute of Physics, Chinese Academy of Sciences)

Presenter: WANG, Lei (Institute of Physics, Chinese Academy of Sciences)

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