# Property directed generative design of inorganic materials

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A combination of AI, high-throughput experiments (robotics) and high performance simulations can be used to accelerated materials development. For inorganic crystalline materials, structure determines property. Therefore, property-driven generative design, driven by machine learning, critically requires understanding of the structure of materials. A deep understanding of crystal structures and their symmetries is essential for accurate generative design.

Thus, the development of symmetry-aware generative models becomes critical to ensure property-directed learning branches. Further, generated crystal structures require validation, both computationally and experimentally. First, I will introduce a generative design framework (WyCryst) [1], composed of three pivotal components: 1) a Wyckoff position based inorganic crystal representation, 2) a property-directed VAE model and 3) an automated DFT workflow for structure refinement. We successfully reproduce a variety of existing materials for both ground state as well as polymorphic structure predictions. We also generate several new ternary materials not found in the inorganic materials databases, which are proved to be stable, retaining their symmetry, and we also check their phonon stability, using our automated DFT workflow highlighting the validity of our approach. We believe our symmetry-aware WyCryst takes a vital step towards AI-driven inorganic materials discovery. Next, we address the challenge of experimental synthesis of these materials paired with data-driven characterization techniques to assess their properties. This is challenging due to the lack of a general method to rapidly synthesize and (optimally) dope bulk materials. We invented a rapid self-sintered solid-state synthesis technique (tested on GeTe, Copper, Silver Antimony Telluride), achieving phase-pure crystalline materials synthesized in the milligram scale in as little as 15 seconds. This accelerates the solid-state reaction process by a factor of >100 relative to the traditional route of mix-and-bake and produce direct experimental validation.

## References

**[1]** Ruiming Zhu, Wei Nong, Shuya Yamazaki, Kedar Hippalgaonkar, WyCryst: Wyckoff Inorganic Crystal Generator Framework, https://arxiv.org/abs/2311.17916 (accepted in Cell Press Matter)

## Figures

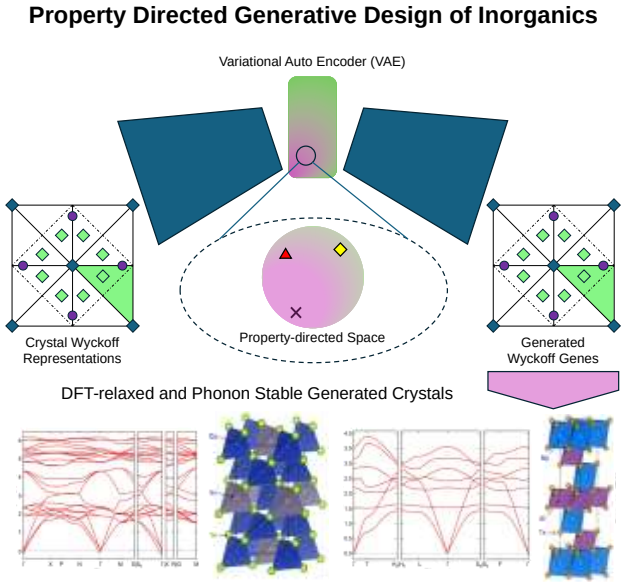


**Figure 1.** Wyckoff based Variational AutoEncoder for generative design