Generative AI models for property to structure materials prediction

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The rapid progress of Artificial Intelligence (AI) models and the increasing availability of large open data sets of computationally predicted materials properties opens new possibilities to design novel materials for sustainable technologies. Over the past decades materials development has increased in speed by orders of magnitude, from the early experimental methods – to simulations based on physics calculations – to AI methods utilizing available datasets. Interaction potentials based on AI models are now part of the standard techniques for materials simulations and have greatly expanded the reach of theoretical prediction and characterization. Previous advances by Goodall *et al.* [1], presents a crystal structure → property prediction AI model approach to high throughput screening of possible crystal structures (see figure 2), increasing the speed for materials development and discovery compared to previous ab-initio physics calculations. The key idea in Re. [1] is the coarse-grained approach using Wyckoff position representation, making the otherwise infinite search space of atomic coordinates enumerable. However, even with these methods — at a computational effort order of magnitudes below prior techniques — the vast size of the chemical and structural space (the combinatorial wall) of even just crystalline materials, makes it intractable to address the general inverse design problem (properties → crystal structure) via brute-force screening of candidate materials.

We develop novel Generative AI (Gen-AI) models that starts from a set of materials properties and generate structural and chemical information to yield a crystalline material, illustrated in figure 1, in an approach that bypasses the combinatorial wall encountered in other screening efforts. The Gen-AI approach in figure 1 can be viewed as a direct search to a crystal structure with the sought materials properties, compared to the previous works in figure 2 where a model can crawl a space of all possible structure inputs and predict properties for each input until the sought set of properties is found. One type of considered models are the diffusion models, which is a family of models that have multiple areas of application [2]. By using the Wyckoff position representation as the structural information, the model is created as a forward process and backwards process as illustrated in figure 3. In the backward process the model is guided towards the sought properties using a classifier in each step. The forward process applies noise that distorts the Wyckoff positions until there is only noise left. In the backwards process, a model is trained to predict a slightly less distorted Wyckoff representation of a structure. Using the backwards process, a Wyckoff representation of a crystal structure can be generated from noise. The generated structure has a high probability to exist due to the nature of the training data. However, in the unguided backwards process, the generated crystal structure can have any materials properties. Thus, the backwards process is guided using a classifier to predict the probability that the slightly less distorted crystal structure has the sought set of properties.

References

[1] Rhys E. A. Goodall, Abhijith S. Parackal, Felix A. Faber, Rickard Armiento, and Alpha A. Lee, *Rapid discovery of stable materials by coordinate-free coarse graining*. *Sci.Adv.* **8**, eabn4117(2022). DOI: 10.1126/sciadv.abn4117

[2] Ling Yang, Zhilong Zhang, Yang Song, Shenda Hong, Runsheng Xu, Yue Zhao, Wentao Zhang, Bin Cui, and Ming-Hsuan Yang. 2023. *Diffusion Models: A Comprehensive Survey of Methods and Applications*. ACM Comput. Surv. 56, 4, Article 105 (April 2024), 39 pages. https://doi.org/10.1145/3626235

Figures

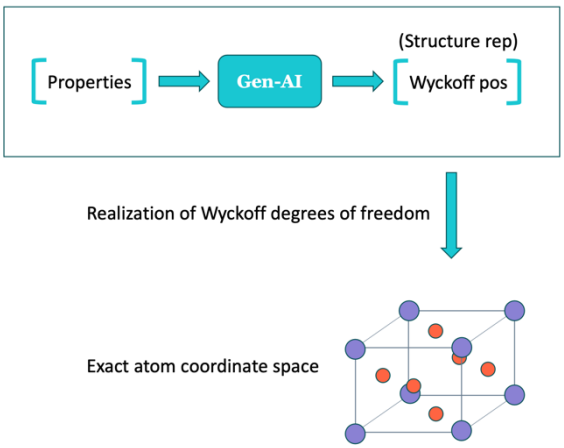

Figure 1. Generative Artificial Intelligence (Gen-AI) model. The model takes a set of materials properties as input and predicts a structure in a Wyckoff position representation corresponding to the input set of properties. Finally, the Wyckoff positions are realized within the degrees of freedom of the Wyckoff coordinates into the exact coordinate space of the atoms, which holds the given sought set of materials properties.

Previous Machine Learning (ML) progress:
Structure-to-Property (S→P) model.
Principle: Crawls space of all possible structure inputs and predicts properties
Benefit: Accelerates traditional ab-initio simulation

Figure 2. Crystal structure to materials properties prediction model for high throughput screening of an enumerable space of crystal structures in a Wyckoff position representation. The model crawls the space of all possible structures as inputs and predicts the materials properties.

Forward process: Apply noise (distortion) on a structure data until only noise left

$$x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_T \sim N(0, I),$$

$$x_0 = "Wyckoff\ representation"$$

Backwards process: Train a model $f_\theta(\hat{x}_{i+1})$ to predict the slightly less distorted structure $\hat{x}_i$ data given the more distorted data sample $\hat{x}_{i+1}$

$$\hat{x}_0 \leftarrow \cdots \leftarrow \hat{x}_{T-1} \leftarrow x_T$$

Figure 3. Description of the principle of the unguided diffusion model process. The forward process in the top applies noise to a Wyckoff position representation of a crystal structure until there is only noise left. The backwards process in the bottom consists of training a model that predicts a slightly less distorted structure until there is a viable crystal structure that has no noise.