

## Inverse Design Framework for Exploring Material Spaces Integrated with Structure Prediction

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We present an inverse design framework for the discovery of inorganic materials using low-dimensional and reversible periodic descriptors[1] derived from the periodic table. Unlike approaches that focus on improving predictions for existing materials, our method enables exploration of chemical spaces beyond known databases.

Motivated by the observation that screening known materials using trained property models often fails to identify candidates that outperform those in the training set, we introduce a periodic descriptor-based exploration strategy to search for new, uncharted compositions. This approach generates promising formulas that are likely to exceed the performance boundaries of existing materials as shown in Fig. 1.

To support structure-aware validation, we constructed classification models for space group and Pearson symbol using approximately 150,000 experimentally reported compounds from the AtomWork-Adv. (AWA) database [2], developed by NIMS. These models enable structure prediction from formula-only inputs, thereby facilitating downstream simulations and structure generation.

### References:

- 1) Y.-J. Wu, Y. Xu, L. Fang, W. Peng, K. Sakaushi, M. Zhang, M. Arai, Y. Koyama, STAM Methods, 2513218 (2025), DOI: 10.1080/27660400.2025.2513218
- 2) AtomWork-Adv., NIMS, 2018. Available from: <https://atomwork-adv.nims.go.jp/>