Structure Prediction from Chemical Formula Using Periodic Descriptors

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Recent advances in machine learning and generative models have opened new opportunities for exploring novel functional materials. However, many of the proposed candidates, especially those generated through formula-based searches, lack structural information, posing a bottleneck for simulation and experimental design. In this study, we explore the potential of our previously proposed periodic descriptors [1], which are low-dimensional and chemically structured features derived from the periodic table, for predicting crystal structure directly from chemical formulas.

We construct classification models trained on approximately 150,000 experimentally reported inorganic compounds from the AtomWork-Adv. (AWA) database [2] to predict structures, including space groups and Pearson symbols. Our models achieve top-3 accuracies of ~0.70 for space group and ~0.76 for Pearson symbol classification. These results demonstrate that compositional patterns captured through periodic trends can be effectively linked to structural tendencies, enabling prototype structure inference.

We further compare our models with benchmark classification tools and analyze prediction consistency across structure classes. This approach addresses the challenge of missing structural data in early-stage materials screening and provides a simple, composition-only method to guide structural assumptions for novel candidates. Future applications will apply this method to newly generated formulas from chemical space exploration algorithms. Structure prediction prior to simulation or experimental evaluation will support a more integrated inverse design framework in inorganic materials discovery.

References:

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2) AtomWork-Adv., NIMS, 2018. Available from: https://atomwork-adv.nims.go.jp/