Structure Prediction from Chemical Formula Using Periodic Descriptors: Toward Inverse Design of Inorganic Materials

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The discovery of novel functional materials increasingly relies on data-driven approaches, yet many formula-based candidates generated through exploration or generative models lack structural information. This absence of structure poses a significant bottleneck for both simulation and experimental planning. In this work, we examine the potential of periodic descriptors [1]—compact, chemically structured vectors derived from the periodic table—for predicting crystal structure types directly from chemical formulas.

Classification models were trained on approximately 150,000 experimentally reported inorganic compounds from the AtomWork-Adv. (AWA) database [2]. The models achieved top-3 accuracies of ~0.70 for space group and ~0.76 for Pearson symbol, and top-5 accuracies of ~0.72 and ~0.87, respectively. These results show that periodic descriptors capture compositional patterns linked to structural tendencies, enabling prototype inference even without geometry information.

We further benchmarked our models against conventional classification tools and analyzed prediction consistency across structure families. This study demonstrates how composition-only models can guide structural assumptions for unexplored formulas, serving as a practical pre-screening step in materials discovery. Future developments will integrate this framework with formula-based exploration and property models, supporting a more complete inverse design workflow for inorganic materials.

References

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