A Crystal's Perspective in Graph Space

A Kernel-Based Machine Learning Approach to Crystal Structures

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Abstract

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In graph theory, a graph provides a natural way to represent interactions within a system, where vertices correspond to atomic sites and edges encode their relationships. This perspective is particularly useful for describing materials whose properties are governed by complex local environments. GraphDot enables the transformation of structures from real space into graph space, where similarities between atomic configurations can be quantified through kernel-based graph dot products. In this work, we apply this framework to crystal structures, focusing on high-entropy alloys composed of five atomic species. By mapping these systems into graph space, we construct kernel matrices that serve as input for machine learning models, allowing us to systematically analyze structural similarity and stability across a wide compositional space.

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