

## Structural database of kagome intermetallics: topology + geometry approach

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The properties of materials are controlled by an interplay of their structure and composition.<sup>[1,2]</sup> The existence of extensive well-curated crystallographic databases allows the identification of materials compositions containing specific structural motifs that determine critical properties.<sup>[3,4]</sup> Accurate identification of materials containing selected extended motifs will strengthen our ability to connect chemical composition to those structural elements that control properties and identify materials whose performance could be improved by further compositional control. The intricate interplay between structure and properties is exemplified by compounds with kagome layers that exhibit a variety of exotic physical states, in particular in intermetallic phases: correlated electron orders,<sup>[5]</sup> topological properties,<sup>[6]</sup> superconductivity<sup>[7]</sup> etc.

Two prevailing approaches have previously been applied to identify materials with such layers: evaluation of topology or geometry assessment, however, both present limitations if applied individually. We augment topological screening with geometrical filtering to allow versatile control over the selection of desired layers. This approach together with the minimal number of other constraints results in the identification of over 9000 intermetallics containing kagome layers.<sup>[8]</sup> These entries are assigned to four classes of structures, revealing the connection between symmetry, structure and composition. These correlations were built into a machine learning model for the prediction of new element combinations that should favour the formation of kagome layers. Some of the highest-ranked phase fields correspond to known kagome-containing materials that were absent from the training dataset, demonstrating that the workflow can identify chemistries affording the target structural motifs and motivating extension of this approach to other extended fragments identifiable with the topology then geometry approach.

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