

## Unsupervised Knowledge Discovery in 'Big' Materials Data

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A major objective in recent computational materials research has been the search and discovery of novel materials with superior properties. However, prior to the availability of immense computational power, materials design was guided by conceptual frameworks for synthesis-structure-property relationships, such as Pauling's Rules, the Hume-Rothery Rules, Pettifor Tables, Structure Maps, Ashby Tables, *etc.* Not only can these heuristic frameworks point us towards new and valuable materials, they also provide a satisfying conceptual foundation upon which to base our scientific intuition. In this talk, I will discuss how we can leverage unsupervised machine-learning algorithms to extract new heuristic relationships from modern large-scale materials databases. In order to extract meaningful synthesis-structure-property relationships, we will first need physically-relevant materials features. Many relevant materials features are not immediately available in current materials property databases. Determination of which features to construct will likely rely on domain knowledge and physical intuition, at least in the near-term future. We will demonstrate how these computational materials discovery and informatics tools can be used to survey, visualize, and explain stability relationships across the inorganic ternary metal nitrides [1].

1. W. Sun et al., "A map of the inorganic ternary metal nitrides", *Nature Materials* (2019)

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