

Abstract Submitted
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Informatics guided Search for Magnetic Apatites PRASANNA V. BALACHANDRAN, TURAB LOOKMAN, Los Alamos National Laboratory — Materials with apatite crystal structure have applications ranging from biomaterials to electrolytes for solid oxide fuel cells. Their chemical flexibility and structural diversity provide a fertile ground to tune functionalities as potential candidates for many applications. However, magnetic apatites are rare. In this work, we use machine learning methods to rapidly screen a vast chemical space and identify novel apatite compositions with magnetic ions. We first construct a database of known materials from surveying the experimental literature. We then augment the database with features that capture the trends in geometry and bonding characteristics of apatites. Supervised classification learning form the basis of our machine learning approach through which we uncover design rules that enable prediction of potentially stable magnetic apatite compositions, prior to experimental synthesis. Finally, we validate our predictions using density functional theory calculations.

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