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AB2(O/F)6 Compounds and the Stabilization of Trirutile[1] RUINING ZHANG, EMILY SCHUELLER, YUZKI HEY, WILLIAM ZHANG, RAM SESHADRI, University of California, Santa Barbara, KYLE MILLER, JAMES RONDINELLI, Northwestern University, METALS AND INSULATORS THROUGH STRUCTURAL TUNING COLLABORATION[2] — The properties of crystalline materials tend to be strongly correlated with their structures, and the prediction of crystal structure from only the composition is a coveted goal in the field of inorganic materials. However, such predictions normally rely on a complex network of interactions and the orthodox methoddensity functional theories calculationsdespite its accuracy, involve high computational and time toils. This research investigates the effectiveness of machine learning methods for structure prediction and searches for new potential compounds. Specifically, we focus on the AB2(O/F)6 composition space with the goal to predict new compounds in the trirutile family. Machine learning methods reduce the time and computational expenses of the search by narrowing down the range of compounds for which density functional theory (DFT) calculations are performed. We predict 18 candidates, previously unreported trirutile oxides. We attempt to prepare two of these and show they form in the disordered rutile structure. Additionally, we develop an understanding of how geometric and bonding constraints determine the crystallization of AB2(O/F)6 compounds in the trirutile structure as opposed to other ternary structures in this space.

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[2]A collaboration between UCSB and Northwestern University.

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