

The Discovery and Design of Multifunctional Materials: Integration of Database Searching and First Principles Calculations

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As technological advances in device syntheses continue to accelerate at an increased rate, there arises an overwhelming need for multifunctional materials. In this talk, we will discuss the development of strategies for the integration of crystallographic database searching with high-throughput first-principles density functional methods for the discovery and design of novel multifunctional materials. We will focus upon recent studies of ternary ABC compositions, of which the most well-known examples are the half-Heusler family, and how this had led us to the discovery of a potential new class of ferroelectrics that is based upon an underdeveloped, previously overlooked family of known materials.