Solid-state synthesis planning from an *ab initio* perspective

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DFT is widely used to predict structure-property relationships for materials design, but the Schrodinger equation provides little guidance on how to actually synthesize newly-predicted materials. Here, I will show how we can guide solid-state synthesis planning using information that is largely-available in high-throughput materials databases like the Materials Project. First, I will discuss a conceptual strategy to navigate high-dimensional convex hulls in the search of reactive precursors for more-efficient materials syntheses. Using a high-throughput robotic synthesis laboratory, we design novel precursors for 32 target quaternary oxide materials, and show that our DFT-guided precursor selection is substantially better for synthesizing the target oxides than naïve traditional precursors. Next, I will show that the onset temperature of a solid-state reaction derives from the extension of liquidus curves into the metastable eutectic region of a Temperature-Composition phase diagram. In order to predict this metastable eutectic temperature, I will present a strategy to combine DFT convex hulls with CALPHAD approaches to rapidly estimate the high-temperature liquidus curves of phase diagrams with minimal computational cost.