A prototypical example based on our current work is shown in Fig. . In Fig. -A we show predictions of the relative stabilities of different oxide polymorphs of . Rutile is most stable, but Columbite is close in stability suggesting epitaxial stabilization may be feasible. In Fig. -B we show computational predictions of a catalytic property for different polymorphs of several metal oxides. The results are not specific to in this example, and are shown to illustrate the approach. In this figure the blue square at the top of the volcano represents the most active polymorph of (Anatase). In Fig -C we show experimental evidence that Columbite can be synthesized on grains that are oriented in the ([100]) and ([010]) directions, but not on grains oriented in the ([001]) direction, which favors the Rutile structure.

This work will not be limited simply to predictions of stability and activity. We will also develop physics and chemistry based models for these properties based on the electronic structure calculations of the oxides (we have been active in this area for the past five years1–8). We will also consider the reactivity of dopant atoms in “metastable” structures7. For example, it may not be possible to synthesize pure Anatase or , but it may be possible to grow epitaxially stabilized solid solutions of Anatase and or to achieve superior properties.

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