Center for Next Generation of Materials Design (CNGMD)
EFRC Director: William Tumas
Lead Institution: National Renewable Energy Laboratory
Class: 2014 – 2020

Mission Statement*: To dramatically transform the discovery of functional energy materials through multiple-property search, incorporation of metastable materials into predictive design, and the development of theory to guide materials synthesis****.***

To realize the *Next Generation of Materials Design*, we will couple first-principles theory with state-of-the-art high throughput and directed synthesis and characterization, including novel *in-situ* methods to understand and predict structure, properties, and phenomena at the molecular, nano, and meso scales. Our current work is focused on three key science questions: 1) How to quantify the synthetically accessible limit of metastability for a number of general synthetic approaches; 2) How to predict synthetic pathways to produce high-energy polymorphs; and 3) How functionality and synthetic pathways can be defined for new multinary oxides and nitrides originating from crystalline and amorphous precursors.

Accordingly, the goals of the CNGMD EFRC are:

Goal 1: Design and discover new energy-relevant materials *with targeted functionalities by integrating theory, high-throughput computation, synthesis, and characterization.* This integrated approach to accelerating materials design and synthesis incorporates both multi-property design and inclusion of metastable materials.

Goal 2: Incorporate metastable materials *into Materials by Design and establish an understanding of metastability including composition, and structure and formation energies for polymorphs and semiconductor alloys.* We will specifically investigate classes of metastability relevant to inorganic semiconductors for optoelectronic applications including polymorphism, semiconductor alloys, and thermochemically metastable compounds***.***

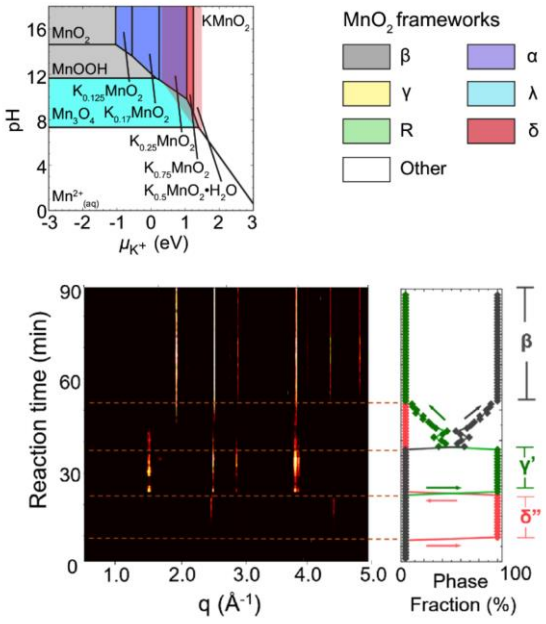

Fig. 1: Top - Predicted pathways for MnO_2 polymorph synthesis. Bottom – Phase formation during synthesis measured using *in situ* x-ray diffraction.

Goal 3: Advance predictive synthesis science *for stable and metastable functional materials by coupling calculated energetics, intermediate structures, and reaction parameters with experimental observables and in situ measurements for 1) aqueous synthesis, 2) solid-state synthesis, and 3) synthesis from amorphous precursors.* We seek to understand the thermodynamics of intermediate states (e.g., nucleation) as well as transient and local conditions (e.g., high chemical potentials of species established by decomposition of reactive precursors) to explain how the materials in Goal 2 can be achieved.

Goal 4: Promote and disseminate *the Next Generation of Materials Design to the broader materials science community*. This includes making our methodology and data accessible as well as organizing conference symposia and workshops.

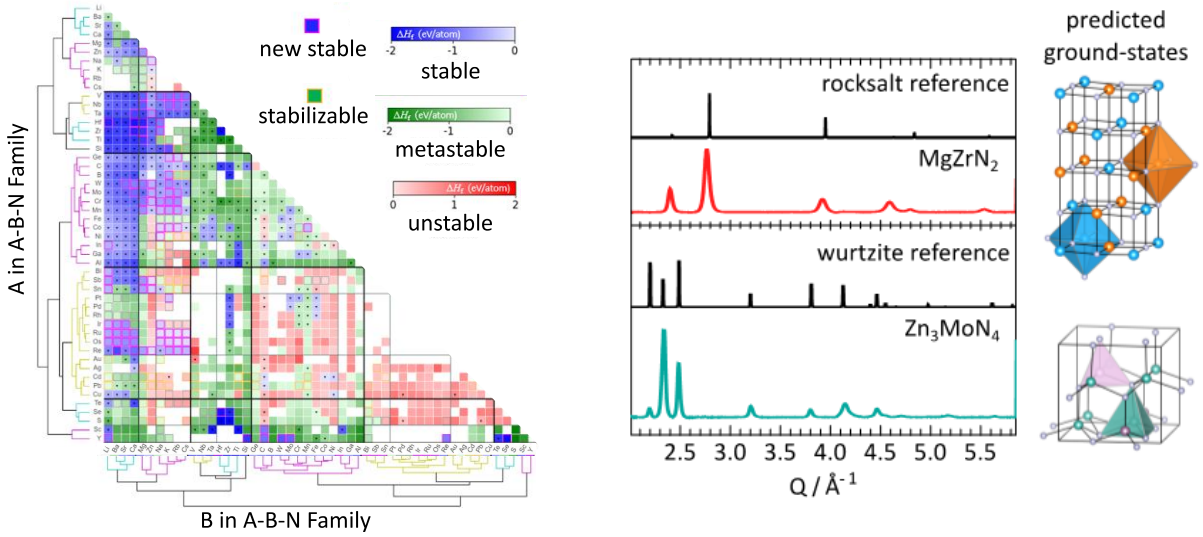

Fig. 2: Left - Map of the inorganic ternary metal nitrides colored by the thermodynamic stability. Right - Predictive synthesis of new ternary nitride functional materials.

Our materials focus is on semiconductors for solar energy conversion, solid-state lighting, power electronics and related technologies—all areas in need of transformative materials. Our current work focuses on two key thrust areas:

Thrust 1: Predictive Synthesis of Complex Metal Oxides will use aqueous and solution-phase synthesis as well as synthesis from amorphous precursor films. We will focus on controlling the synthesis of high energy polymorphs and functional ternary metal oxides.

Thrust 2: Nitride Materials will focus on understanding and controlling nitride metastable materials and metastable heterostructural nitride alloys.

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