

Center for Next Generation of Materials by Design (CNGMD): Incorporating Metastability
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Lead Institution: National Renewable Energy Laboratory
Start Date: August 2014

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 by 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. This EFRC is specifically designed to address several critical scientific gaps that must be overcome before computational materials design becomes a robust tool delivering new functional materials — namely 1) **multiple-property design**, 2) **accuracy and relevance**, 3) **metastability**, and 4) **synthesizability**. This approach will expand and accelerate the discovery of accessible materials for energy applications.

The Center for Next Generation of Materials by Design (CNGMD) EFRC aims to discover and synthesize novel functional materials including non-equilibrium structures in a predictive manner. Accordingly, the five 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 incorporates both multi-property design and the inclusion of metastable materials.
- **Goal 2: Develop foundational tools for theory, synthesis, and characterization to enable the next generation of Materials by Design,** including theoretical methods for rapidly predicting atomic and electronic structure, novel *in-situ* characterization, and high-throughput synthesis and characterization techniques.
- **Goal 3: Incorporate metastable materials into Materials by Design and establish an understanding of metastability including composition, structure and formation energies for polymorphs, semiconductor alloys and defects.** We will specifically investigate four broad classes of metastability relevant to inorganic semiconductors for optoelectronic applications: polymorphism, semiconductor alloys, defects, and thermochemically metastable compounds (Fig. 1).
- **Goal 4: Develop theory-driven synthesis approaches to guide synthesis of new materials, including metastable systems, by coupling theory and state-of-the-art in-situ characterization to probe materials growth pathways.** 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 3 can be achieved.
- **Goal 5: Promote and disseminate the Next Generation of Materials by Design to the broader materials science community.** This includes making our methodology and data accessible as well as organizing conference symposia and workshops.

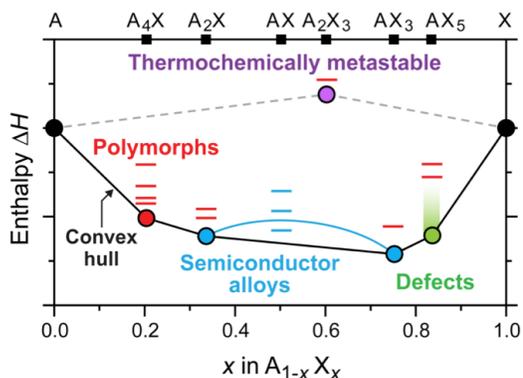


Fig. 1: Four classes of metastability being addressed by CNGMD.

Our materials focus is on semiconductors for solar energy conversion, solid-state lighting, power electronics and related technologies—all areas that need transformative materials. Our current work includes six research projects (P1-P6) as well as outreach activities and foundational tool development.

- **P1: Pnictide Search** integrates theory and experiment to discover new semiconducting nitrides, a relatively unexplored class of materials, most of which are inherently metastable. SnN, a new metastable binary nitride, has been realized.
- **P2: Polymorphs and Synthesizability** takes a multipronged approach combining theory and experiment to predict, synthesize and explore synthetic pathways to specific polymorphs. Initial focus is on Mn, V and Ti oxides as exemplary polymorphic materials. We have developed *Polymorph Sampler*, a new first-principles approach to predict polymorph stabilities and distributions.
- **P3: Chalcogenide Alloys** uses first principles calculations to predict alloy phase diagrams for realizing new functionality. New features have been found to emerge in heterostructural alloys compared to conventional isostructural alloys. This has been demonstrated in the SnCaS and MnZnO systems (Fig. 2).
- **P4: Defect Phase Diagrams** integrates theory and experiment to explore the nature and energetics of complex defects in creating functional materials. The effective electronic doping of wide-gap Ga₂O₃ has been achieved.
- **P5: Perovskite-Inspired Materials Search** identified defect tolerance and long carrier lifetime as the key features of the hybrid organic-inorganic halide perovskite photovoltaic absorbers. Based on the resultant design principles, nine new classes of potential materials have been identified and five new materials with desired properties have been demonstrated.
- **P6: Piezoelectric Materials Search**, a new project started in 2016, is developing Pb-free piezoelectric materials, including theoretically predicted but previously unsynthesized metastable materials. Two such materials have been realized.

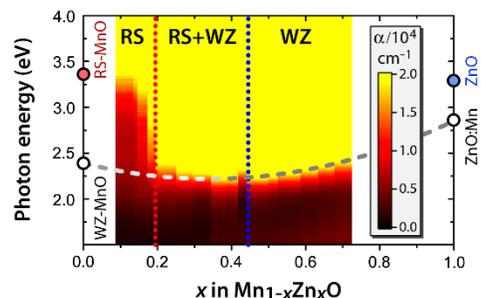


Fig. 2: Measured absorption coefficient α (contour plot) and calculated band gaps (dashed line) for Mn-Zn-O alloys.

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