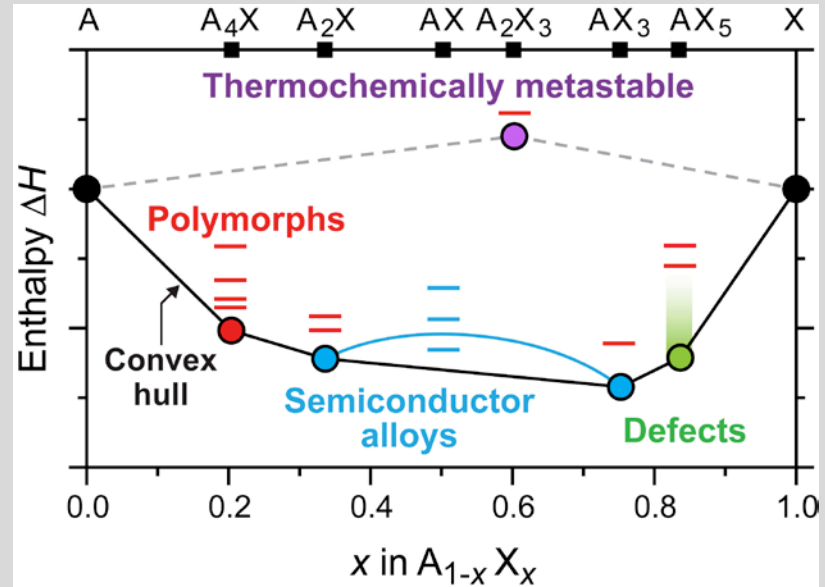


Center for Next Generation of Materials by Design (CNGMD)

William Tumas (National Renewable Energy Laboratory)

The mission of the Center for Next Generation of Materials by Design is to dramatically transform the discovery of functional energy materials through high-throughput multiple-property searching, incorporation of metastable materials into predictive design, and the development of theory to guide materials synthesis.

www.cngmd-efrc.org



Four classes of metastable materials (shown in color) targeted for theory-driven synthesis in the CNGMD EFRC.

RESEARCH PLAN

- Integrate high-throughput theory, experiment, and data mining to develop a rapid search and design methodology for *discovery of new functional materials*.
- Develop new tools to accelerate materials discovery incorporating *metastable semiconductors: polymorphs; defects, disorder, interfaces; & alloys*.
- Predict *synthesis pathways* by coupling theory and *in-situ* characterization.



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