

Attachment 1 – Research Topic Template

1. **Research Title:** Predicting Phase Stability in Chemically Complex alloys
2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level**

Materials Science, Physics, Computer Science (MS, PhD level)

4. **Objectives:** Employ first principles methods to predict the equilibrium phases over a range of temperatures for chemically complex alloys outside the range of conventional CALPHAD databases.
5. **Description:** Compositionally complex alloys (e.g. High Entropy Alloys) contain high concentrations of three or more elements. Often the target compositions are outside the range of existing phase diagram databases. Predicting the desired phases and their volume fraction using CALPHAD methods then becomes a highly inaccurate extrapolative process. Recent work has shown that a set of micro canonical assemblies can be used in conjunction with ab initio Monte Carlo methods to sample a wide range of possible equilibrium ground states that may contain one or more phases. Here these techniques, and possible extensions, are applied to a wide range of compositionally complex refractory-metal alloys. Such methods accelerate the initial sampling of a wide range of alloys compositions and can be used to inform CALPHAD methods.
6. **Research Classification/Restrictions:** This research topic is basic research and will be published in the open literature.
7. **Eligible Research Institutions:** Indicate to what organizations this topic should be provided

DAGSI (Wright State University, AFIT, Ohio State University, University of Dayton, Miami University, Ohio University, University of Cincinnati) NOTE: Topics submitted to DAGSI must be approved for public release. Need PA Approval #

AFIT (only)