**Opportunity Title:** Designing entropy-stabilized oxides: A stochastic, first principles-finite temperature approach
**Opportunity Reference Code:** ORNL-HBCU-MEI-2019-0008

**Organization** Oak Ridge National Laboratory (ORNL)

**Reference Code** ORNL-HBCU-MEI-2019-0008

**How to Apply** All documents must be submitted via Zintellect. All application components **must** be completed and received in the system in order to be considered.

***Application deadline January 11, 2019 at 11:59 pm EST.***

For questions, please contact HBCUMEI@orau.org.

**Application Deadline** 1/14/2019 11:59:00 PM Eastern Time Zone

**Description** ORNL is the largest science and energy laboratory in the Department of Energy system. Areas of research include materials, neutron sciences, energy, high-performance computing, systems biology and national security. Visit http://www.youtube.com/watch?v=NSCdUJ8cavw to discover some exciting reasons why ORNL offers a great internship experience!

**Benefits:**

- Selected faculty spend 10 weeks (Summer Term) at Oak Ridge National Laboratory (ORNL) engaged in a research project under the guidance of a laboratory scientist.
- Faculty members build collaborative relationships with ORNL research scientists, become familiar with ORNL sponsored research programs, scientific user facilities, and potential funding opportunities.
- ORNL may provide laboratory tours, scientific lectures and seminars, workshops on accessing ORNL scientific user facilities.
- Host laboratories provide all required site specific training.

**Project:**

The overarching goal of this proposal is the first principles predictions of finite temperature behavior of chemically disordered materials. We aim to develop a scalable, efficient, first-principles approach for studying finite-temperature properties by combining the stochastic Wang-Landau method with density functional theory (DFT) energetics. As proof of principle, we will investigate entropy-stabilized oxides, a relatively new class of materials where five chemically disordered elements on the cation sublattice result in a unique phase transition driven by configurational entropy. The Wang-Landau method offers a promising solution for the examination of temperature-dependent properties defined by ensemble averages, yet has largely been applied to lattice models with discrete basis sets, e.g. Ising or Potts models. We will (i) adapt this approach to explore finite-temperature properties with energetics taken directly from DFT, (ii) develop tools to extract kinetic information from the simulations and (iii) use experimental synthesis and characterization for validation and, in conjunction with machine learning techniques, to bridge the gap between end member information and solid-solution structural stability. Of interest, will be first principles predictions of structural phase transitions, melting temperatures and thermal conductivity for potential applications. We anticipate that the framework developed will be fundamental for extending DFT above 0K, ground state predictions with wide-ranging applicability across numerous materials systems.

**Faculty Mentor/Point of Contact (email address):** Valentino R. Cooper coopervr@ornl.gov

**Qualifications** **Applicant must be a faculty member at a HBCU/MEI at the time of application.**

Familiarity with first principles, density functional theory methods. Applicants with experience in stochastic approaches such as the Monte Carlo and/or Wang-Landau approaches are encouraged. Emphasis will be placed on chemically disordered materials that undergo unique temperature-dependent phase transitions.

**Eligibility Requirements**

- **Citizenship:** LPR or U.S. Citizen
- **Degree:** Master's Degree or Doctoral Degree.

- **Discipline(s):**
  - **Engineering** (27)
  - **Mathematics and Statistics** (11)
  - **Nanotechnology** (1)
  - **Other Physical Sciences** (12)
  - **Physics** (16)

**Affirmation** I am a faculty member at one of the nationally recognized HBCU or MEI institutions. I can provide certification of my faculty position, if requested.