2023 INCITE Proposal Submission
Proposal

Title: Ab Initio Investigation of Disorder and Defects in Structural and Functional Materials

Principal Investigator: Markus Eisenbach

Organization: Oak Ridge National Laboratory

Date/Time Generated: 6/17/2022 3:14:07 PM

Section 1: PI and Co-PI Information

Question #1

Principal Investigator: *The PI is responsible for the project and managing any resources awarded to the project. If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.*

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Question #3

Institutional Contact: *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

Institutional Contact

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Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Materials Science: Condensed Matter and Materials

Question #2

Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)

Project Summary

Real materials show disorder at the atomic level and behave differently from perfect crystals that can be described readily with standard computational methods. We employ high performance computing to explore the quantitative and qualitative changes in the behavior of electrons in materials due to disorder and finite temperature that can lead to new fundamental behavior.

Section 3: Early Career Track

Question #1

Early Career

Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an Early Career Track in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.

***Who Can Apply**: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

How to Apply:

In the regular application process, there will be a check-box to self-identify as early career.

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.

- *What is the Early Career Track?*
  - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
  - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
  - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.*
- *What review criteria will be used for the Early Career Track?*
  - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.

No

If 'yes', what year was your PhD? If 'no' enter N/A

N/A

If 'yes', how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.

N/A

Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Node Hours

290,000

Storage (TB)

2

Off-Line Storage (TB)

2

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

250,000

Storage (TB)

2

Off-Line Storage (TB)

2

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Node Hours

460,000

Storage (TB)

2

Off-Line Storage (TB)

2

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

Node Hours

560,000

Storage (TB)

2

Off-Line Storage (TB)

2

Question #5

ALCF Theta (Cray XC40) Resource Request - 2023

Question #6

ALCF Polaris Resource Request - 2023

Question #7

ALCF Polaris Resource Request - 2024

Question #8

ALCF Polaris Resource Request - 2025

Question #9

ALCF Aurora (Intel X^e) Resource Request – 2023

Question #10

ALCF Aurora (Intel X^e) Resource Request – 2024

Question #11

ALCF Aurora (Intel X^e) Resource Request – 2025

Question #12

List any funding this project receives from other funding agencies.

Funding Sources

Funding Source

DOE BES

Grant Number

ERKCS92

Funding Source

DOE BES

Grant Number

ERKCS91

Funding Source

DOE BES

Grant Number

ERKCK47

Funding Source

DOE BES

Grant Number

ERKCS81

Funding Source

NSF

Grant Number

1931367, 1931445, and 1931525

Funding Source

NSF

Grant Number

2103598

Question #13

List any other high-performance computing allocations being received in support of this project.

Other High Performance Computing Resource Allocations

Resource

NERSC

Allocation Agency

DOE Office of Science

Allocation

7,000

Allocation Year

2022

Section 5: Project Narrative and Supplemental Materials

Question #1

Using the templates provided here, please follow the INCITE Proposal Preparation Instructions to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file. Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.

Concatenate all materials below into a single PDF file.

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

INCITE_2023_25_Proposal-full.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: Ab Initio Investigation of Disorder and Defects in Structural and Functional Materials

PI and Co-PI(s): Markus Eisenbach (ORNL), Valentino R. Cooper (ORNL), Mina Yoon (ORNL), Swarnava Ghosh (ORNL), Ka Ming Tam (LSU), Hanna Terletska (MTSU), Yang Wang (CMU)

Applying Institution/Organization: Oak Ridge National Laboratory

Number of Node Hours Requested: 2023: 290,000 (Summit), 250,000 (Frontier); 2024: 460,000 (Frontier) 2025: 560,000 (Frontier)

Amount of Storage Requested: 2 TB

Executive Summary:

The goal of this project is to gain a first principles based, quantitative understanding of the role of disorder and defects in alloys and functional materials beyond the ideal, ordered, zero temperature ground state. To achieve this goal, we will combine density functional theory based *ab initio* calculations with statistical mechanics methods and first principles data driven models. The calculations for disordered materials, statistical sampling of configuration distributions and the generation of first principles data for model generation share as common features a high level data dependent stochastic part and a compute intensive deterministic kernel, that will allow the exposure of multiple levels of parallelism, scaling towards the exascale.

In this project we will investigate partially overlapping classes of important materials that are significant from both a basic science point as well as for their potential technological applications. Thus we will focus on the statistical physics and functional behavior of high entropy alloys and high entropy oxides, magnetic functional materials with spin-orbit interactions that lead to complex spin order (skyrmions) and quantum states (topological insulators and Weyl semimetals) and disorder driven phenomena in photovoltaic semiconductors.

Solving the problems related to the first principles understanding of real materials poses challenges that require extraordinary computational capabilities. While the ground state properties of some pure compound can readily be calculated, real materials with defects and impurities and complex magnetic configurations have to be considered. This makes the calculation of even the ground state for realistic models containing approximately 100k atoms a petascale problem. Including finite temperature properties, disorder fluctuations or electron correlation in these materials requires orders of magnitude more computational resources. Finite temperature effects will be modeled by sampling the energy landscape with the Wang-Landau (WL) statistical approach. The value of the energy at the sampled points will be determined by the Locally Self-consistent Multiple Scattering (LSMS) method and the well established FHI-aims code will be used for verifying our results. The efficiency of WL sampling, the scalability of LSMS, and the computing power of Summit (and Frontier in coming years) combine to allow a truly first-principles thermodynamic description of disordered functional materials. Furthermore, by combining the first principles results with our newly developed machine learning workflows, the capabilities of this computational approach can be extended to explore wider ranges of material compositions and external parameters with existing computational resources.

In addition to these calculations, that are well supported by our existing codes, we will develop new capabilities, in the form of dynamical mean field theory, that will allow us to explore the interplay of electron correlation and disorder.

PROJECT NARRATIVE

1 SIGNIFICANCE OF RESEARCH

This project aims to advance the understanding, from first principles, of the role that statistical fluctuations and defects have for the behavior of alloys and functional materials. We will achieve this goal by applying combined computational and data driven methods to the materials design and quantitative understanding of alloys and functional quantum materials. The area of materials design of alloys requires the understanding of many levels of physical phenomena ranging from the electronic level, accounting for chemical and magnetic effects, through defect kinetics, incorporating atomic transport, to dislocations and grain boundaries, leading to high level and macroscopic properties. In this project, we will apply first principles and data driven approaches to address the behavior of materials from the ground up and provide important references for first principles based atomistic design of structural and functional materials for a wide range of applications.

As a key foundation to achieve this goal, we will perform an extensive set of first principles large cell calculations for multi component materials, based on our past work on steels and high entropy alloys (HEAs). To be fully predictive, such an approach must be based on first principle calculations which make it applicable to any arbitrary chemical compositions. Accurate prediction demands data obtained from calculations for large supercells, $> 10^3$ atoms, which is well beyond standard, small supercells, $\approx 10^2$ atoms, accumulated in traditional first principle datasets. This is crucially important for disordered materials to capture the relevant statistical, fluctuation-influenced interactions affecting their behavior.

This INCITE allocation will provide computer resources to enable research in the Materials Theory, Modeling and Simulations Section at Oak Ridge National Laboratory, that is funded by the following DOE-BES awards: *Advanced Theoretical and Computational Approaches for Quantum Materials* (ERKCS92, PI: F. Reboredo), *Simulation, Design, and Discovery of Complex Materials* (ERKCS91, PI: V. R. Cooper), *Understanding and Controlling Entanglement in Solid-State Systems via Atomic Scale Manipulation* (ERKCK47, PI: S. Jesse), *Growth Mechanisms and Controlled Synthesis of Nanomaterials* (ERKCS81, PI: K. Xiao), and Quantum Science Center at ORNL. Further efforts involved in this proposal are part of the MuST project supported by NSF Office of Advanced Cyberinfrastructure and the Division of Materials Research within the NSF Directorate of Mathematical and Physical Sciences under award number 1931367 (Terletska), 1931445 (Tam), and 1931525 and 2103958 (Wang).

The main computational packages we will use for the proposed research projects are 1) MuST/LSMS, which is developed by the PIs at ORNL and in a NSF funded CSSI project as a public *ab initio* electronic structure software package and 2) FHI-aims, both with petascale and beyond computing capability, for first principles study of quantum phenomena in disordered materials.

In this project we are pursuing four aims: 1) The structural understanding of chemical disorder in high entropy alloys (HEA) and high entropy oxides (HEO), 2) the influence of disorder on the magnetic state of functional materials, 3) disorder-driven electron localization and its importance for photovoltaic materials, and 4) the large scale calculations of correlated materials with disorder.

1.1 High Entropy Alloys and Oxides

For material sciences, the prediction of alloy phase transitions is of paramount importance. The understanding of order-disorder transitions in metallic materials has been a longstanding problem with important technical implications. It is obvious that predicting and mapping the phase diagram of a material will be useful for designing new materials, the ordering of intermetallic compounds is crucial for their mechanical properties, as ordering in intermetallics contributes to the extreme brittleness at low temperatures. The unique properties of high entropy alloys (HEA) [1] depend on their chemical disorder, that has to remain

stable against ordering or phase separations at sufficiently low temperatures. These alloys contain a large number of elements at approximately equal atomic concentrations. This has for the most part hindered the development of reliable, effective interatomic potentials that could be used in classical model simulations using molecular dynamics of Monte-Carlo methods. Thus, it is highly desirable to perform direct first principles simulations of the chemical order in HEAs as a function of temperature to determine their thermodynamic stability. This will be complemented by data driven workflows for automated machine learning model refinements for classical statistical mechanics simulations.

Several experimental studies in recent years have revealed that the arrangement of atoms in HEAs is not ideally random due to the diversity in atomic sizes and the complex interactions between the constituent elements which usually result in structures with short-range order (SRO) during solidification or/and heat treatment processes. As a result, observation of SROs and their possible effects on the mechanical and physical properties have drawn much research attention lately in the study of HEAs. Recent experiments [2, 3] have shown that SRO has significant effects on the deformation behavior of HEAs, suggesting that tuning the degree of SROs is an effective way for optimizing mechanical properties of HEAs.

In 2015, the discovery of the entropy stabilized oxides added a new family to the class of high entropy oxides. By mixing MgO, CoO, NiO, CuO and ZnO it was found that $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ (hereafter MgO-HEO) could be stabilized in a rock-salt structure in which the cations are fully disordered [4]. The entropy stabilized oxides are not only interesting from a fundamental scientific point of view as this entropy-driven stabilization may engender many unique properties, such as high melting temperatures, radiation resistance and other anomalous responses. But also have a wide variety of promising chemical, thermal, and electrical properties, similar to that of the aforementioned HEAs [5]. Recent neutron experiments performed at ORNL have reported that bulk MgO-HEO displays antiferromagnetic (AFM) order. This discovery is remarkable, given the extreme disorder induced by the randomly distributed moments of Co, Ni and Cu and the 40% of spin vacancies created by the nonmagnetic Mg and Zn ions. Studying these materials requires identification of the relevant competing phases and structures as well as the response to external factors such as magnetic/electric fields and temperature.

The thermodynamic stability of a crystal structure versus competing phases (e.g. structures with different stoichiometries or chemical elements) is directly related to whether a particular material can be grown as a single phase and, thus, the extent to which the expected properties can be obtained. Evaluation of stability needs a detailed analysis of the energetics of the relevant competing compounds. For complex multicomponent structures, somewhat standard approaches like the special quasirandom structure (SQS) method [6] have helped to reduce the computational costs, but still offer only limited views of the configurational landscape. This failure is embodied in the difficulties in evaluating the entropic contributions, S, within a material's phase space. One approach has been to employ data mining and machine learning on data extracted from experimental databases to predict random, homogeneous multicomponent compounds. However, these efforts rely heavily on the availability and quality of experimental databases and are often limited to metal alloys. Naturally, such approaches have been adapted to take input from first-principles calculations, and have seen some success. Nevertheless, these approaches still suffer from the large computational cost of electronic structure methods that ultimately lead to an undersampling of the configurational landscape.

Previously, we employed a bond enthalpy model, based on first-principles calculations to examine the relative stability of different phases of a five-component high entropy oxide [7]. Using this model approach, combined with Metropolis Monte Carlo simulations we were able to simulate the temperature-dependent phase fractions that would be present in this compound. Interestingly, with such a simple model, that only had knowledge of the first neighbor metal atoms, we were able to accurately observe the transition from a multi-phase compound, to a single homogenous, fully disordered material. Remarkably, our results were able to identify a "hidden phase" that was potentially missed in the original experimental X-ray character-

ization due to overlapping Bragg peaks. More recently, we were able to demonstrate that this approach is fruitful for explaining the short-range order observed from neutrons for five-component pyrochlores [8].

In this project, we propose to use a stochastic approach, the Wang-Landau (WL) method, combined with direct DFT energy evaluations to explore chemical, temperature and pressure dependent properties of multicomponent oxides. We aim to extend the predictive power of DFT beyond ground state properties. A key component of the research will be the use of binary oxide enthalpy of mixing maps to extrapolate the local bonding energy. This will require us to first build a database of enthalpies of mixing for different cation combinations across a large number of different crystal structure types.

This will then be the basis for Wang-Landau Monte-Carlo simulations of cation mixing and segregation. Using this approach, we will be able to examine the relative phase fractions of the different structure types as a function of temperature and pressure in appropriate sized simulations cells with some built-in information of local distortions. This will be crucial for exploring the large phase space of these compounds and will be used in the next phase of this project. To illustrate its value, we will simulate entropy-driven phase transitions in oxide solid solutions; primarily focusing on mechanical properties, related to thermal stability and defect dynamics, as well as magnetic behaviors in these materials with broad applicability in fields including piezoelectrics, molecular crystal structure prediction and liquid-solid interfaces, like those involved in catalysis and gas absorption.

1.2 Magnetic and Quantum Functional Materials

Magnetic order is of significant interest for functional materials and the design of spintronic devices. The magnetic structure of a material is determined by the interplay and balance of their electronic structure, exchange interactions, spin-orbit coupling, and for long range order, magnetostatics. We will thus explore the capabilities to control the magnetic behavior of materials by conducting first principles calculations that provide a detailed analysis of the influence of doping and defects that gives rise to changes in these fundamental interactions. We will address fundamental research questions in materials that exhibit reduced local symmetries due to the underlying crystal lattice, heterostructures, defects and disorder. The crystal field may alter the occupation of localized electrons in the d orbitals. Reduced symmetry highlights the importance of spin-orbit coupling effects for the behavior of these materials. Heterostructures, such as multilayers, hold the promise for designing materials by tuning magnetic interactions, like the Dzyaloshinskii-Moriya interaction and dipolar interactions that can stabilize topological magnetic structures such as skyrmions [9].

The physics of skyrmion lattices is fascinating not only from the perspective as an emerging non-trivial topological object, but also because long living stable skyrmions represent potential candidates for spintronics materials. The basis of the skyrmion lattice formation is the long period magnetic structure [10, 11]. The parent ferromagnetic coupling (J) with the non-inversion symmetric Dzyaloshinskii-Moriya (K) interaction form a ground state with helical spin structure. The wavevector of this helical structure is determined by the ratio of the K/J. Under the magnetic field applying along the <001> direction, the spiral structure deforms into a conical structure. Various mechanisms of stabilizing this phase have been proposed. In particular, classical Monte Carlo simulations have demonstrated the formation of skyrmions in a simple model [12]. However *ab initio* studies are proven to be rather challenging. This is mainly due to the large period of the spiral structure arising from the small Dzyaloshinskii-Moriya coupling compared to the ferromagnetic coupling. Thus, the theoretical understanding of the spin structure in chiral magnets and the competition between different phases has been largely based on classical spin simulations as the size of these structures has been beyond the reach of most first principles methods. Thus, first principles computations of skyrmions have been attempted only recently [13]. LSMS [14], as a linear scaling *ab initio* method, is perfectly suited for the calculation of magnetic structures with large unit cells, which are necessary for the simulation of skyrmion lattices. In particular, since the spin-orbit coupling, as a relativistic effect, plays an essential role

in the formation of skyrmions, the relativistic LSMS provides a rare opportunity to study skyrmion lattices, which has hitherto been difficult, if not impossible, for other *ab initio* methods.

Another class of recently discovered functional magnetic materials are the magnetic topological insulators. Topological insulators (TI) have been extensively studied for more than a decade, with *ab initio* analysis been proven to be an important computational tool to describe such systems [15, 16]. Magnetic ordering which explicitly breaks the time reversal symmetry can be induced in topological insulators by magnetic dopants [17]. This induces the opening of a gap in the surface states and leads to exotic quantum phenomena, such as the anomalous Hall effect [18]. TI are characterized by gapless topological boundary states which have a Dirac-cone like dispersion and are protected by time reversal symmetry. The introduction of magnetism in the TI can introduce a gap in the topological boundary states, which lead to exotic topological phenomena such as axion insulator states [19], quantum anomalous Hall (QAH) effect [18], magnetic Weyl semimetals [20] and topological magnetoelectric effects [21].

3D topological insulators of the Bi_2Te_3 family have been used as a platform to realize these exotic phenomena [22, 23], for example, QAH effect in V and Cr doped Bi_2Te_3 and Sb_2Te_3 thin films [24, 18, 25]. $MnBi_2Te_4$ is a layered compound which was first proposed theoretically and later realized experimentally to be the first intrinsic magnetic topological insulator. In $MnBi_2Te_4$, septuple layers of Te-Bi-Te-Mn-Te-Bi-Te is stacked through van der Waals interactions along the c-axis. At temperatures below 25 K, each septuple layer is ferromagnetic (FM), which align antiferromagnetically (AFM) with the neighboring septuple layers. The number of septuple layers in thin films of $MnBi_2Te_4$ tunes the magnetism. A thin film of $MnBi_2Te_4$ with a single septuple layer is ferromagnetic, an even number of septuple layers give rise to compensated AFM, and an odd number gives rise to uncompensated AFM. Furthermore, the magnetism can also be tuned by external fields. As the magnetic ground state of these compounds can be engineered, a wide variety of topological phenomena such as Chern insulators, axion insulators, AFM TI, and type-II Weyl semimetals have been experimentally realized. Experimentally synthesized $MnBi_2Te_4$ includes disorder such as Mn on Bi or Bi on Mn antisite defects. Such defects, though present at low concentrations, have been observed to influence the magnetic ground state of this compound. Furthermore, addition of dopant atoms, such as Cr and V, can also be used to tune the magnetism.

Delafossite, which forms an ABO_2-type crystal structure, is another quantum material with rich functional properties [26]. The material consists of alternating planes of A (cation) layers and (distorted) BO_6 octahedra, where A and B comprise a wide range of elements in the periodic table, leading to diverse and unconventional physical and chemical properties [27]. For example, it can be a p-type semiconductor, a Mott insulator, a quantum material with unconventional anomalous Hall effect, and so on. On the other hand, it is challenging for material synthesis, so only a few materials with high-quality crystals have been synthesized so far. We plan to use our computational approaches to understand their properties and stability to support experimental efforts to synthesize new functional quantum materials with improved properties.

1.3 Photovoltaic Energy Materials

A dramatic effect of disorder in materials is Anderson localization, when electron scattering off random impurities leads to their spatial confinement within a finite region of space, and hence limits their contribution to transport [28]. Such disorder-driven localization of electrons has been found to be essential for tuning the functional properties of intermediate band semiconductors, the promising candidates for the efficient energy harvesting solar cells [29, 30]. Unlike conventional solar cell materials, intermediate band semiconductors have a partially filled impurity band located between the valence band and the conduction band. This provides an extra channel for the promotion of an electron from the valence band to the conduction band by absorbing two low energy photons instead of one with the energy of the whole band gap. To be relevant for efficient solar cell operation, the intermediate band must be delocalized and conducting [31]: enabling a

two-step harvesting process of photons.

Disorder can be used to control such localization of charge carriers in the intermediate band, and therefore, to manipulate the photovoltaic properties of the system. In semiconducting materials, the level of localization of states on the impurity band is sensitive to the level of doping. It has long been a challenging problem due to the large supercell required for small doping concentrations, usually on the order of 1% or less. Significantly larger cluster sizes than those accessible by conventional supercell methods are required. Hence, leveraging the LSMS large-scale supercell capabilities is necessary for a proper theoretical description of electron localization in such systems [14].

1.4 Large Scale Calculations of Correlated and Disordered Systems

The properties of real materials are strongly influenced by electron-electron interaction and disorder [32]. In particular, both correlations [33] and disorder [28] are two possible mechanisms behind the metal-insulator transitions in quantum systems [34]. Due to the non-perturbative nature, understanding the combined many-body effects of electron interactions and disorder in materials is a challenging task [35]. The problem has, thus, attracted great interest by a wide variety of methods, although still much remains to be learned. Recently, much progress has been achieved in incorporating correlation effects within *ab initio* studies using DFT-based computational approaches [36]. Methods which combine DFT and other approximations to account for the strong correlations have been proposed over the past three decades. The most widely used one is the DFT+U method for which an extra energy contribution from the local interaction is included in the static energy shift [37]. A more elaborated method which incorporates the correlations effects and the dynamical nature of the interaction is the dynamical mean field theory (DMFT) [35]. Here, the many-body effects are treated exactly at the quantum impurity level in an accurate self-consistent way.

In this project, we aim to explore the correlations and disorder effects using the large-scale LSMS approach, that would allow us to address the existing numerical challenges of other *ab initio* methods. Conventional plane wave-based DFT calculates the eigenfunction and eigenenergy of the Kohn-Sham equations, and requires a down-folding procedure for constructing the Green's function as the input for the DMFT [36, 38]. As an alternative, accurate self-consistent methods for solving the Kohn-Sham equations based on the local density approximation (LDA) in terms of Green's functions have been developed within the multiple scattering theory-based KKR approach [39]. One of the biggest advantages of the KKR-DMFT approach is that it is a Green's function-based approach, and hence it bypasses the difficulties in down-folding used in DFT-based band-structure methods. Another appealing feature of the KKR-DMFT approach is that it also allows for the incorporation of disorder effects into the analysis [40, 39, 41]. Hence, using the KKR-DMFT approach within our LSMS framework opens an avenue for studying the interplay of electron-electron interactions and disorder in real materials (Sec: 2.4), such as functional semiconductors and disordered alloys.

1.5 Previous INCITE awards

1. 2008–09, Petascale Simulation of Strongly-Correlated Electron Systems Using the Multi-Scale Many-Body Formalism
2. 2010–12: Magnetic structure and Thermodynamics of Low Dimensional Magnetic Structures
3. 2013–15: Scalable first principles calculations for materials at finite temperature
4. 2016–17: First principles based statistical physics of alloys and functional materials
5. 2018–20: First principles investigation of solid state phase transitions
6. 2021: Disorder and statistical mechanics of alloys and functional materials
7. 2022: Large Scale Simulation of Disorder in Alloys and Materials

2 RESEARCH OBJECTIVES AND MILESTONES

2.1 Chemical Ordering in Alloys and Oxides

In this project we will investigate important classes of materials, where the understanding and control of ordering has both fundamental and technological applications. The desire is to find systems where the chemical ordering of the atomic species on the underlying crystal lattice can be suppressed, as in high entropy refractory alloys and high silicon content steel. In both cases, we will be performing LSMS [42, 43] calculations to find the order-disorder phase transition for fixed concentrations and to generate reference data sets that map configurations to energy (and magnetic order in the case of magnetic materials). These data sets, which will be made available, form the input to our machine learning workflow to fit efficient surrogate model Hamiltonians that will be used for further Monte-Carlo simulations of these materials.

In conventional metals, defects such as vacancies, dislocations, stacking faults and twins disrupt the local structure, but in HEAs, they also disrupt the local chemistry. This makes investigation of kinetics and energetics of defects very challenging. Unlike conventional metals where strengthening results in loss of ductility and toughness, certain characteristics of twin and phase boundaries in HEAs make them less brittle when strength is increased. These attractive features make HEAs suitable for applications needing stronger and tougher materials.

In metals, the Generalized Planar Fault Energy (GPFE) curve depicts the energy barriers for various fault structures and can be used to understand the energy landscape corresponding to the nucleation of dislocations, twin formations and subsequent migration of boundary planes. This energy landscape is also influenced by pre-loading stress. In year 1, we propose to calculate the GPFE curves for Cantor (specifically, the CoCrFeMnNi single phase alloy and its derivatives) and refractory HEAs for different cases of short range ordering parameters and pre-loading stress. In year 2, we will use WL-LSMS to simulate the finite temperature properties of dislocations in Cantor and refractory HEAs and in year 3 we will focus on finite temperature properties of twin and grain boundaries in HEAs.

High entropy refractory alloys are an important research area in the design of alloys for high temperature applications that have been dominated in the past by Ni-based superalloys. We will explore this class of materials using WL-LSMS calculations and by constructing surrogate models using our Uncertainty Quantification based machine learning workflow[45, 44] that will be used within Monte-Carlo simulations. Fig. 1 show our results of this data-riven approach for MoNbTaW. We will explore 5-component and 6-component refractory concentrated solid solution alloys, by considering equal concentrations of additional metals which neighbor MoNbTaW in the periodic table. Using this approach, we will establish the stability of concentrated solid solution HEA phases in these materials as well as the evolution of short range order at finite temperature.

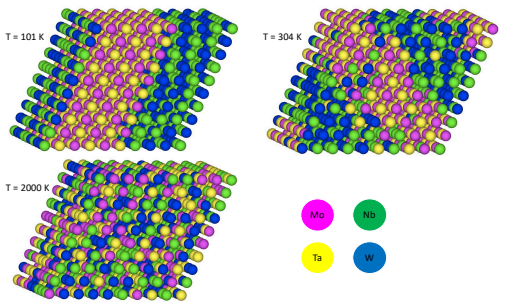

Figure 1. Snapshots of the structure of MoNbTaW at 101 K, 304 K, and 2000 K. [44]

The second research topic in this project is high entropy oxides, built on our initial work focused on simulating the temperature-dependent phase transitions in 2- to 5-component oxides comprised of MgO, CoO, NiO, CuO and ZnO. In this project, we will explore the structure, stability, and functionality of multicomponent ceramics. The goal will be to discover which combination of metal cations and stoichiometries can be stabilized and how these metastable phases can induce new functionality. For example, we will examine the possibility of enhancing the piezoelectric and magnetoelectric couplings in perovskites; which have long

been a fruitful playground for tuning ferroic couplings (i.e., couplings between magnetism, polarization, and elastic behaviors). In this framework, d0 cations, which are favorable for driving ferroelectricity, can be paired with magnetic cations that typically do not form perovskites with large polar distortions. The challenge will be to find suitable combinations that retain magnetic ordering and sufficiently larger polar distortions in a stable, single phase perovskite. This work will leverage our prior efforts to examine the local, disorder-induced macroscopic crystallinity in multicomponent relaxor oxide ferroelectrics [46, 47]. Similarly, building on our recent work examining the phase stability of pyrochlores [48], we will extend our approach to examine other complex multicomponent oxides, such as the spinnel class of materials, to ascertain which combinations of metal cations may promote homogenous, single phase materials. This work will be in collaboration with experimental efforts within ORNL in crystal growth and characterization, particularly as it applies to materials for energy storage devices. One intriguing feature of high entropy oxides is the potential for tuning the barriers for ion motion. This can be exploited to either enhance such motion for battery technology or to reduce the motion to make them radiation resistant. In the realm of structural materials, we have already demonstrated that in the *A*O high entropy oxides, the isotropy of the elastic properties is intimately related to magnetism as well as the presence of additional phases [49]. This suggests that temperature and magnetic fields may be unique knobs for tuning the elastic and perhaps thermal properties of these materials. We will continue to investigate similar materials to better understand these phenomena.

In addition, we will study the influence of disorder in the exchange couplings on the spin-wave excitations in multicomponent oxides, like the MgO-HEO. This will be done in two stages. In the first stage, we will use the abovementioned procedure to examine the stability of different *A*-site cations in MgO-HEOs and pyrochlores to screen potential materials for emergent behaviors. Subsequently, we will examine magnetic exchange couplings within these materials. In particular, we will examine the role of non-magnetic ions and disorder on magnetic frustration within these materials. In some multicomponent compounds, the distribution of non-magnetic ions could potentially lead to regions of the material in which the density of magnetic ions may be below the percolation threshold needed to sustain magnetism. Coupled with the potential for ferromagnetic interactions between some ions and antiferromagnetic interactions with others, it is anticipated that some mild magnetic frustration may emerge. Indeed, moderate frustration, expressed as the ratio of the Curie-Weiss temperature over the Néel temperature, has been reported for MgO-HEO [5]. Such frustration due to nearest neighbor interactions could explain some of the other curious magnetic properties of MgO-HEO, such as the broad phase transition ranging from 100 to 140 K, the persistence of spin-wave excitations up to room temperature, and the bifurcation of the field-cooled and zero-field-cooled magnetic susceptibility. Here, we will examine the effects of replacing non-magnetic ions with magnetic ions and vice-versa, to understand the frustrated magnetism in these materials. We will further explore routes to enhance the coupling between magnetism and other degrees of freedom; potentially "dialing" the magnetic and polar phase diagram to engender unique multiferroic properties.

This work will have a twofold purpose. First, it will provide a fertile playground for testing our framework combining DFT and Monte-Carlo calculations for studying the finite temperature, dynamic behaviors of materials. We will employ our modular, scalable workflow which allows us to easily interface WL simulations with atomic structure codes and machine learned potentials (OWL [50]). Using such potentials (parameterized from DFT calculations) we will simulate the multi-to-single phase transition observed in entropy-stabilized oxides. Following this, we will also employ OWL with direct DFT energetics. A practical outcome of the WL+DFT approach will also be the generation of a dataset that could be used to reparametrize less expensive empirical potentials; thus, allowing for larger (length and time) scale studies like the effects of defect motion at grain boundaries on structural stability. This database will also provide a foundation for future machine learning attempts to identify new entropy stabilized ceramics. Additionally, direct WL+DFT simulations should allow us to get more accurate predictions of phase transitions within these systems. Such predictions and their correlated local atomic order will be validated by neutron scatter-

ing pair distribution functions (PDFs) and x-ray diffraction studies. Similar theory-experiment comparisons were instrumental in understanding the subtle differences between the PDFs obtained for PZT at different compositions and the underlying local structure origins of the observed macroscopic phases [51].

2.2 Magnetism in Functional Materials

Materials with crystal structures without inversion symmetry, such as the B20 structure or nanostructured materials, provide intriguing complex magnetic spin textures that arise from the competition of exchange and spin-orbit interactions [10]. The lack of inversion symmetry gives rise to antisymmetric exchange or Dzaloshinskii-Moria interactions. Skyrmions are topological magnetic defects, and recently the energy barrier for the formation and destruction of skyrmion lattices in MnSi has been measured using small angle neutron scattering [52]. The discovery of skyrmion lattice phase in the MnSi presents a breakthrough in the search for spintronics materials. Unfortunately, computer simulations of skyrmion lattice present a challenge as the magnetic structure of skyrmion is usually very large. For example, the MnSi skyrmion size is about 20nm [53]. Even for the simulation of the magnetic structure of a single skyrmion, the size of the supercell required is well beyond the capability of plane wave DFT. We have the unique capability to further this research by utilizing our LSMS. Using fully relativistic calculations, including spin-orbit coupling, we will investigate these low symmetry magnetic materials, in particular the effect of defects and disorder on the magnetic interactions. Our calculations will focus on the effect that chemical substitutions have on the energy barriers of the topological states, and the pinning and depinning of the magnetic texture to the underlying crystal lattice, as has been observed experimentally in Ga substitutions in MnSi [54]. In addition to the large scale first principles calculations, we will employ our data driven machine learning approach to construct surrogate models to be used in MC simulations of the magnetic behavior of these topological magnetic systems. These calculations will provide insight into the formation and stability of topological spin order, which usually are only stable in restricted volumes of phase space and will allow us to incorporate fluctuations of magnetic interactions due to chemical order into the understanding of these materials.

In year 1 we will focus on the mechanisms of magnetic ordering in MnGe [55]. There are two main advantages for the LSMS and multiple scattering method for MnGe. First, the skyrmions are relatively small, about 3nm [55]. It may still be an insurmountable challenge for plane wave DFT, however this is well within reach for the LSMS method. Second, there is no energy gap for the materials and thus it does not involve the difficulty in locating the chemical potential.

Another challenge for the *ab initio* method is that the skyrmion lattice does not exist at zero temperature, it is stabilized by both the external magnetic field and the thermal fluctuation [56, 12]. Combining the Wang-Landau sampling and the LSMS with a ML workflow, we can study the systems at finite temperatures. We will calculate the phase diagram of the MnGe as a function of magnetic field and temperature. Focus will be on the magnetic structure in different phases, to characterize the formation of skyrmions, the spin winding number will be calculated. In year 2 we will investigate the MnSi for which a precise calculation of the chemical potential to fix the electron density is required because of the energy gap [57] and finally in year 3 we will include the effect of Ga substitutional disorder in our calculations.

Topological insulators are a class of quantum materials that have gaps in the bulk but metallic edge or surface states, which are protected by time reversal symmetry. Long-range magnetic order in a topological insulator can break the time reversal symmetry, open an exchange gap in the surface states, thereby leading to exotic topological quantum phenomena such as axion insulators [19], quantum anomalous Hall (QAH) effect [18], and magnetic Weyl semimetal state [20].

Manganese Bismuth Telluride ($MnBi_2Te_4$) and Manganese Antimony Telluride ($MnSb_2Te_4$) form an important family of Van der Waals magnets. $MnBi_2Te_4$ is the first experimentally realized intrinsic magnetic topological insulator. It is a Van der Waals compound consisting of septuple layers of Te-Bi-Te-Mn-Te-Bi-

Te stacked along the crystallographic c-axis. At a temperature below 25 Kelvin, the high spin Mn^{2+} ions order ferromagnetically in each septuple layer, and each septuple layer couple antiferromagnetically with its neighbors, thus forming an A-type antiferromagnetic (AFM) structure. $MnSb_2Te_4$ is isostructural with $MnBi_2Te4$. Just like ordinary materials, disorder is also omnipresent in topological insulators. Experimental investigations [58] and theoretical calculations [59] have shown that site mixing between Mn and Sb/Bi ions in $MnSb_2Te_4$ and $MnBi_2Te_4$ can switch the magnetism from AFM state to a ferromagnetic (FM) state. Disorder is present at low concentrations; few parts per million for vacancies to few percent for dopants and site mixing. This makes first principles simulations of defects at realistic concentrations extremely challenging due to the large cell sizes required. The LSMS code can solve the Kohn-Sham equations for thousands of atoms, and therefore can be used to determine the relative energy differences between the different magnetic phases, and the precise concentration of dopants at which the phase transition occurs. The LSMS code can be also used to calculate the pair exchange parameters $J_{ij}(|r_i - r_j|)$, which can be then employed in mesoscale simulations. In Year 1, we will focus on calculating the energies of ferromagnetic, ferrimagnetic and antiferromagnetic states with various concentrations of disorder in bulk $MnBi_2Te_4$. We will calculate the exchange constants J_{ij} for $MnBi_2Te_4$, which will be inputs to Heisenberg Hamiltonian to calculate the Curie temperature, susceptibility and the co-existence of different phases in $MnBi_2Te_4$. In year 2, we will focus on studying the coupling between defects, strain and magnetism in $MnBi_4Te_7$ ($MnBi_2Te_4$+Bi_2Te_3). Finally, in year 3, we will focus on $MnSb_4Te_7$ ($MnSb_2Te_4$+Sb_2Te_3).

Our recent experiments (done by Zheng Gai et al. at CNMS, ORNL) identify different surface terminations of magnetic Weyl semimetal $Co_3Sn_2S_2$. Sulfur adatoms for 1D chains on the CoSn terminated surface and S adatoms located at different positions in the chains show distinguishable electronic property (as identified by STS). We need to understand the formation of different sulfur isomers on the surface (monomer, dimer, trimer, and chains) and their electronic properties. The CoSn terminated kagome lattice displays two different types of vacancies, Sn and Co The Sn vacancy form monomers with three-fold symmetry and they are nonmagnetic. On the other hand, Co vacancies are magnetic, as they show difference with magnetic tips and magnetic fields. First-principles calculations are in need to understand the origin of the magnetic Co vacancy and their three different states observed in experiments.

2.3 Localization in photovoltaic semiconductors

The main purpose of this part of the project is to explore the electron localization in the intermediate band semiconductors (Sec:1.3). With the disorder being a powerful tool for controlling the functional properties of materials, there is a critical need of *ab initio* numerical tools that would enable quantitative treatment of electron localization in real materials. Recently, we have implemented the Lloyd's formula [60] within the LSMS approach, which significantly expands the existing capabilities of LSMS, and allows the treatment of disorder in more relevant and wider range of materials. Within the Lloyd's approach the accurate determination of the Fermi energy is done without numerical integration of the Green's function along the energy contour, which is particularly important for the materials featuring the band gaps.

In year 1, in order to enable the quantitative detection of the electron localized states using the LSMS formalism, we will combine the Lloyd's formula with the typical medium embedding scheme (Sec. 3.2.3). This will allow us to study the electron localization in several families of intermediate band semiconductors. In year 2, we will focus on Si:Ti systems. In [61] combing the typical medium formalism with the Effective Disordered Hamiltonian Method (EDHM) [62], we have shown the mid-gap states in Si:Ti become Anderson localized at doping roughly 0.1%. Our special interest will be on the impact of the charge self-consistency which is present in LSMS, but is absent in EDHM approach. It was shown in [63] that such full self-consistency is important for proper capturing of electron localized states, including other proposed mechanisms of electron localization, such as the Mott screening effects [33]. In year 3, we will investigate the Anderson localization in other proposed intermediate band semiconductors. We will study

V-doped In_2S_3[64], Co-,Ti-, S- doped Si [65, 66, 67] systems. The goal is to determine the critical density of impurities needed to induce the metal-insulator transition. As a result of this study, we will generate a list of theoretically predicted critical impurity concentrations required for the metal-insulator transition in proposed intermediate band materials. This will be valuable for validating the existing theory of electron localization in such materials [31], and possibly will be of use for designing the intermediate band solar cells with improved efficiencies.

2.4 DMFT for Correlated Materials with Disorder

The goal of this part of the project is to study how the properties of materials are influenced by electronic interaction and disorder. Implementing the strongly-correlated DMFT analysis into our MuST/LSMS framework will enable us to perform the large-scale computation of the many-body correlation effects in various quantum functional materials.

The KKR-CPA/LSMS-DMFT formalism also opens the venue to perform an *ab initio* study of materials which possess both *strong* correlation and *strong* disorder effects resulting in electron localized states. We have shown [68, 63] that the Mott transition due to strong correlation and the Anderson transition due to strong random disorder can be captured without bias in such a unified framework. Challenging problems regarding the physics of the competition between Mott insulator and the Anderson insulator, such as the formation of local moment in doped silicon, will be addressed beyond simple models by *ab initio* study.

In year 1, we will incorporate the DMFT formalism within our MuST/LSMS code for large scale calculations. We will follow the procedure outlined in the multiple scattering theory- based formalism of Ref. [39]. As a Green's function method, our MuST/LSMS framework provides a natural connection to the embedded impurity system used in the DMFT. In LSMS, we will be able to perform calculations on a very large Matsubara frequencies grid, and, hence, to explore accurately much wider parameter space in materials.

In year 2,we will incorporate disorder into the DMFT method implemented in the MuST/LSMS framework from year 1. This will allow us to study disordered alloys which find applications in a large number of areas in material science. In our implementation, we will follow closely the KKR-CPA-DMFT implementation of ref. [69], where in addition to KKR-DMFT, the effective medium CPA analysis is included to allow incorporating the chemical disorder effects. First, we will test our formalism by performing analysis for $Cu_{1-x}Pd_x$ binary alloys and half-metallic NiMnSb alloys using the LSMS formalism on a large Matsubara frequency grid, and compare the results against the data obtained using analytical continuation of [69].

In year 3, we will apply the developed KKR/LSMS-DMFT formalism to various correlated and disorder materials of interest. The metal insulator transition in the phosphorus doped silicon is the classic example which suggests that the competition and cooperation between strong correlation from the Mott physics and random disorder should play a crucial role. Another class of semiconductors which has the interplay between strong correlation and random doping is the magnetic semiconductors, such as $Ga_{1-x}Mn_xN$ and $Ga_{1-x}Mn_xAs$. We will then apply the KKR-CPA/LSMS-DMFT to extend our study on magnetic semiconductors [70].

3 COMPUTATIONAL READINESS

We will use different scientific codes to accomplish different milestones as outlined in the milestones table. While the majority of our calculations will utilize our MuST/LSMS code, which implements KKR, KKR-CPA, and LSMS methods, we will also use FHI-aims and, to a smaller extend, Quantum Espresso in combination with our Wang-Landau and machine learning workflows. All the applications and workflows we are planning to use in this project are able to scale to a significant portion of Summit and make use of GPUs for acceleration. The memory requirement for all these codes is small and the on-node memory is adequate. No major data storage and transfer are required.

The MuST/LSMS package is available on GitHub (https://github.com/mstsuite) under a BSD 3-clause li-

cense. As a component of MuST, the WL-LSMS code is written mainly in C++ and FORTRAN. It uses Message Passing Interface (MPI) for massive parallelization, OpenMP for on-node parallelization, and CUDA or HIP respectively for acceleration on NVidia and AMD GPUs. It relies heavily on numerical libraries for linear algebra: BLAS and LAPACK and the accelerator specific implementations in cuBLAS/rocBLAS and cuSolver/rocSolver, and a domain specific library for exchange-correlation functionals: libxc. The I/O requirements will remain modest using HDF5. In addition to these requirements, the KKR and KKR-CPA calculations require SCALAPACK, and the full-potential LSMS and KKR calculations also require FFTW and P3DFFT packages for parallel fast Fourier transform.

3.1 Use of Resources Requested

The resources requested are calculated based on our past experience with OLCF allocations on Summit and preliminary scaling results on Frontier and on estimates of the iteration steps required to calculate the thermodynamic properties by sampling the systems phase space.

In particular the measurements for LSMS for a typical system that can be extracted from the scaling plot provided in this proposal indicate a computational requirement for self-consistent LSMS calculations of 1.4 node-seconds per atom and iteration step. For a typical 1024 atom Wang-Landau LSMS calculation the measured sampling rate corresponds to 18 node-minutes per Monte-Carlo move. While the number of Monte-Carlo steps needed for convergence is not known a priori, our experience is that approximately 0.25M moves are required to reliably calculate a phase transition temperature, which translates to 75,000 Summit node-hours per simulation per system investigated using WL-LSMS. Systems with larger phase spaces will need more MC samples and thus resources to reach the same level of convergence.

For the investigation of disorder and localization effects in doped semiconductors, we will apply the embedded LSMS method to the electronic structure calculations. The entire SCF calculation can achieve high performance by taking advantage of multiple levels of parallelizations: 1) parallelization over N_c atoms; 2) parallelization over N_e energies along an energy contour; 3) parallelization over the angular momentum quantum number (l, m) up to $l = l_{\max}$ when calculating the regular and irregular solutions of the single site scattering; 4) parallelization over N_k points in Brillouin zone integration for the calculation of the effective medium τ-matrix. Therefore, the calculation has a trivial $N_c \times N_e \times \max((l_{\max}+1)^2, N_k)$ fold parallelism. In practice, the parallelization is set up as follows: for P_{T} total MPI processes, it is broken down into three integer numbers P_{A}, P_{E}, and P_{K} with $P_{\mathrm{T}} = P_{\mathrm{A}} \times P_{\mathrm{E}} \times P_{\mathrm{K}}$, so that each process performs calculations for N_C/P_{A} atoms and N_e/P_{E} energy points, and for each energy point, each process calculates $\underline{\tau}(\mathbf{k};\epsilon)$ for N_k/P_{K} $\mathbf{k}$-points and $(l_{\max}+1)^2/P_{\mathrm{K}}$ regular and irregular solutions.

The investigation of doped semiconductors require using large supercells crystal structure to simulate the disorder effects. We expect a typical supercell to contain 16384 atomic sites. Initial tests for 1024 atomic sites shows that each SCF iteration requires 5 node-hours on Summit. Thus, running 100 SCF iterations (expect to be sufficient for convergence) for the 16384 atomic sites requires 8,000 Node-Hours. For each doping type, we consider 5 supercell samples, with a different impurity contents.

3.2 Computational Approach

3.2.1 First principles and Monte-Carlo

We combine first principles calculations with classical Monte-Carlo simulations either directly (WL-LSMS [42, 43]) or using a tightly couples machine learning workflow [44] to sample the physical phase space for finite temperature properties, of which the stochastic, statistical nature provides a natural means for massive scalability. Both approaches use a hybrid parallelization scheme. At the top level, the codes employs concurrent random walkers using a master-worker scheme. The second parallelization level is the first principles portion of the code as described below, thus achieving scalability up to the full size of available

HPC systems. For added sampling efficiency, we utilize the flat histogram Wang-Landau method [71]. It is much more robust than traditional Monte Carlo methods as the simulation is carried out *independent* of temperature, yet the thermodynamic properties at *all* temperature can be calculated at the end of a simulation.

3.2.2 The LSMS Algorithm

The core of our calculations are based on first principles density functional theory (DFT). To solve the Kohn-Sham equations we use a real space implementation of the multiple scattering formalism. This allows LSMS to achieve linear scaling og the computational effort in the number of atoms in the system. The details of this method for calculating the Green function and the total ground state energy $E[n(\vec{r}), \vec{m}(\vec{r})]$ are described elsewhere [14, 72]. The computationally most intensive part is the calculation of the scattering path matrix τ for each atom in the system by inverting the multiple scattering matrix $\tau = [I - tG_0]^{-1} t$. The only part of τ that will be required in the subsequent calculation of site diagonal observables (*i.e.* magnetic moments, charge densities, and total energy) is a small (typically 32×32) diagonal block of this matrix who's rank is $O(4k)$. These dense matrix operations will allow us to employ highly optimized dense linear algebra libraries (BLAS, LAPACK and accelerator equivalent libraries - cuBLAS, cuSolver) to achieve maximum utilization of the on node floating point compute capabilities. Most importantly for the application in the hybrid Wang-Landau LSMS method and for ML surrogate model construction, our Locally Self-consistent Multiple Scattering (LSMS) method [14] allows the possibility of non-collinear magnetism [73]. Since an arbitrary arrangement is not a DFT ground state we will have to deal with a constrained general state [74, 75]. In the constrained local moment (CLM) model the LSDA equations are solved subject to a constraint that ensures that the local magnetizations lie along a prescribed directions prescribed. Thus this method enables the calculation of the energies of arbitrary orientational states as generated by the Wang-Landau algorithm.

3.2.3 Typical medium embedding approach in LSMS

In order to capture the electron localization in real materials, the local interaction zone (LIZ) cluster in the LSMS method must be embedded in the typical medium. The typical medium approach [76] is able to properly account for the non-self-averaging behavior of the disorder induced Anderson localization phenomena and provides a proper order parameter to detect the Anderson localized states. Specifically, across the Anderson transition, dramatic changes of the distribution of the local density of states (LDOS) occur. At small disorder the LDOS has a Gaussian distribution, while it is skewed log-normal distribution at large disorder [68]. To capture such non-self-averaging behavior, the typical medium theory (TMT) approach employs the geometric instead of algebraic averaging over disorder. This typical DOS (TDOS) has been shown to reflect the behavior of the most-probable value of the LDOS across the transition with vanishing TDOS [76], and hence, can be used as an order parameter to identify the Anderson localize states. We have recently implemented LIZ cluster embedding in the typical medium in 3D tight binding Anderson model [61, 77]. In this scheme, the LIZ is used to efficiently compute the local Green's function of a super-cell embedded in a local typical medium. Applying such embedding in the LSMS scheme in 3D Anderson model, we not only find quick convergence with increasing LIZ cluster size, but also obtain an accurate estimate for the critical disorder strength for the Anderson transition [61]. The method has also been tested for a variety of distributions of random disorders. [77] These studies provide a solid foundation for studying electron localization in *ab initio* LSMS framework. Thus, combining LSMS with the typical medium embedding scheme opens the way to study strong disorder effects and electron localization for very large supercells, which are inaccessible to plane wave based DFT methods.

3.2.4 Dynamical mean field theory

Electron correlations play an important in quantum materials. A successful method to account for many of the effects of electron correlations within an *ab initio* theory combines the local density functional (LDA) approximation of density functional theory with a strong on-site Coulomb interaction term U between elec-

trons to reintroduce the correlation effects that are missing in LDA. Dynamical mean field theory (DMFT) in combination with the LDA is capable to solve this problem [78, 38]. DMFT maps the many body problem onto a multi orbital quantum Anderson impurity model. In DMFT the many body interacting Green's function G of the system is calculated from the non-interacting Green's function G_0 by replacing the lattice self-energy with the impurity self-energy. The impurity problem itself is solved using a many body method such as quantum Monte Carlo or perturbative approaches such as fluctuation-exchange theory and the iterated perturbation theory. Since LSMS directly calculates the Green's function of the system, it forms a natural basis to connect to DMFT [39]. While all of the previous implementations of LDA+DMFT have been based on k-space formulations of DFT we will combine it with our real space LSMS method which will enable the efficient, scalable calculation of large correlated systems with defects and heterostructures that are relevant for the discovery of functional quantum materials. As an added benefit, LSMS promises the efficient calculation of the Green's function at sufficiently many complex Matsubara energies that the connection between the DFT calculation and the Anderson impurity solver can be performed without the need for constructing the, numerically problematic, analytical continuation of the Green's function.

3.2.5 Machine Learning

Calculations of material behavior usually has to employ a hierarchy of models ranging from highly accurate, yet computationally expensive, quantum mechanical first principles methods to effective empirical surrogate models that can treat the large length and time scales that are inaccessible to the higher fidelity models. We will utilize data driven Machine Learning (ML) models that enable large scale, high fidelity calculations that bridge the capability gap between different levels of theory. In particular this will allow us to derive effective models of magnetic interactions from DFT calculations that can be employed within our classical Monte-Carlo simulations of finite temperature statistical mechanics. We have recently employed model binary and refractory high entropy alloy systems to develop novel workflows to generate ML surrogate models for these materials that reproduce the DFT results with accuracies that are suitable for statistical mechanics predictions. [45, 79, 44]. Here, we will apply this approach to magnetic systems that will build on our past experience [80] for magnetic interactions to be able to describe the complex chemical order and the magnetic order in the non collinear systems in this proposal.

3.2.6 FHI-aims

Additional first-principles calculations will be performed using the FHI-aims code. FHI-aims is a mature, high-precision, all-electron electronic structure code that makes no shape approximations to the underlying potential. This makes it particularly suitable for the elucidation of properties related to spin-orbit coupling (SOC), which is a relativistic effect and is typically shaped most strongly by the atomic region near the nucleus. The numeric atom-centered basis sets of FHI-aims [81] achieve a high-precision description of the region near the nucleus, as well as precision for total-energy–based properties of molecules and materials on par with the best available benchmark codes. The code covers current density functionals and many-body approaches; and it is particularly strong regarding the scalability of all of its key density functional methods to very large system sizes (thousands of atoms) [82] and on the highest-performance distributed-parallel architectures, while retaining the full numerical precision of all operations. FHI-aims features a a GPU port of key parts of the code. The code has demonstrated scalability on Summit [83].

3.3 Parallel Performance

WL-LSMS is able to make good use of the Summit architecture and major parts have been ported successfully to exploit Nvidia accelerators. The weak and strong scaling of WL-LSMS is near perfect. In addition to the scalability WL-LSMS achieves a high computational efficiency. In the past we demonstrated the performance and scalability of LSMS and WL-LSMS by performing representative test calculations for Fe supercells on Titan using GPUs and comparing the performance to CPU only calculations. [84] Since then, we have ensured that our LSMS and WL-LSMS codes are functional on the Summit and Frontier systems

and we have performed performance and scalability studies to guide our resource request for 2023 through 2025. In figure 2 we compare the strong scaling of LSMS for as small 128 atom calculation in the number of GPUs used. We also show the scaling of Wang-Landau LSMS on Summit with the results shown in figure 3. A straight extrapolation to the full system would yield a sampling rate of 3.7 samples per second on the full Summit system at this choice of 8 atoms per GPU. Finally, we demonstrate the weak scaling and

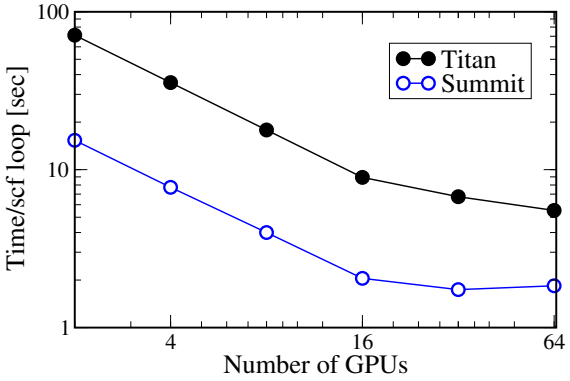

Figure 2. Strong scaling of LSMS for a 128 atom test case on both Titan and Summit from 2 to 64 GPUs. The ratio of execution time for 2 GPUs is 4.6.

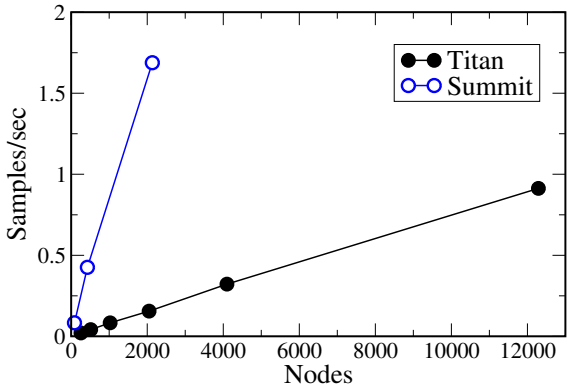

Figure 3. Scaling of WL-LSMS. The Summit run on 2134 nodes (46% of the full system) achieves 1.69 WL samples/sec., (Titan 0.9128 WL samples/sec. on 12289 nodes - 66% of Titan).

the capability of a single LSMS instance to run across all of Summit. In figure 4 shows the capability of LSMS to scale from 3 nodes on Summit to 4500 nodes (98% of the full machine) for a self-consistent first principles density functional calculation of 216,000 Fe atoms.

As LSMS is one of the Center for Accelerated Application Readiness (CAAR) codes for the OLCF Frontier system (https://www.olcf.ornl.gov/caar/frontier-caar/), we have worked with the system vendors and OLCF to improve the performance on Frontier. This has allowed us to obtain early scaling and performance measurements on Frontier. In figure 6 we show the weak scaling of FePt calculations from 2 nodes to 4096 nodes with 64 atoms per node (8 atoms per GPU). For comparison we show the time on Summit for a single node with the same number of atoms per GPU. Additionally we also have early strong scaling results for 65,536 and 131,072 atom systems on Frontier. These results indicate that, together with the CAAR improvements in LSMS, we can, at present, expect an $\approx 5.5\times$ per node speedup on Frontier when compared to Summit.

FHI-aims has a strong history of parallel performance and has been used in production on many leadership class computing systems. Of central importance for the present proposal is cross-node parallel performance including GPU use. Our recent publication demonstrates GPU algorithms and performance of the present code on multiple architectures (Intel/NVidia and Power/NVidia), for multiple generations of NVidia hardware. As a key example of the extent of scalability achieved with the present status in FHI-aims, in Figure 5 we show data for a topological insulator, a Bi_2Se_3 slab consisting of 375 Bi and Se atoms as a benchmark system. For the runs with GPUs, we used one GPU per MPI task.

3.4 Developmental Work

3.4.1 Embedded LSMS

The implementation of embedded LSMS is currently under development, led by Yang Wang in collaboration with Markus Eisenbach, Hanna Terletska, and Ka Ming Tam. Terletska and Tam will provide guidance on the computational algorithms for calculating the typical medium that the LIZ is embedded in. Eisenbach will provide guidance on high performance computing and numerical calculations on Summit. Wang will implement the calculation of $\underline{\tau}_{\text{Med}}(\mathbf{k};\epsilon)$, $\underline{\boldsymbol{\tau}}_{\text{Med}}(\epsilon)$, $\underline{\tau}^{nn}(\epsilon)$, and the Lloyd formula in MuST.

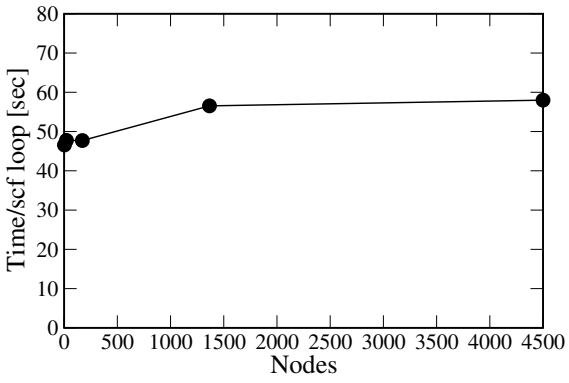

Figure 4. Weak scaling of LSMS on Summit using GPUs. From 3 nodes for 128 atoms to 4500 nodes (98% of the full machine) for 216,000 atoms.

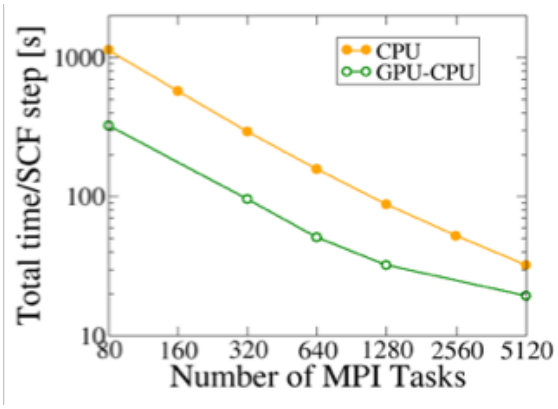

Figure 5. Benchmark calculation showing a strong scaling of FHI-aims on Summit for a Bi_2Se_3 slab with 375 Bi and Se atoms.

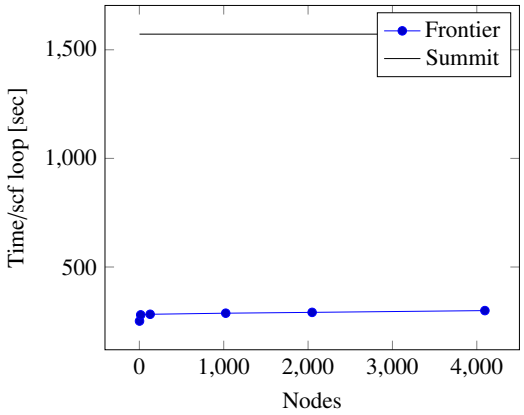

Figure 6. Weak scaling of LSMS for FePt ($lmax = 7$) with 64 atoms per node from 2 to 4096 Frontier nodes.

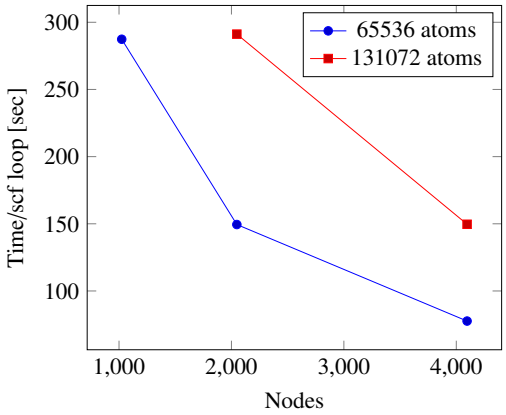

Figure 7. Strong scaling of LSMS for FePt ($lmax = 7$) from 1024 to 4096 Frontier nodes.

3.4.2 Dynamical Mean-Field Theory

We will implement DMFT in our LSMS code for large scale calculations. As a Green's function method our MuST/LSMS framework provides a natural connection to the embedded impurity system. The self energy needs to be evaluated for $\approx$ 4000 Matsubara frequencies. As the LSMS approximation improves for large imaginary parts, the Green's functions can be evaluated without need for analytical continuation.

3.5 Development plan for next-generation systems

We continue to improve our MuST/LSMS code and ensure its portability and performance on future HPC architectures. As a significant computational effort of our multiple scattering codes is based on complex dense linear system solvers on a single node, we expect the continued performancebased on vendor provided libraries for the BLAS and LAPACK equivalent functionality. Additionally, we are implementing accelerator kernels for portions of our code that have not yet been ported to accelerators, such as the single site solvers, calculation of observables and energies and the construction of the potentials.Additionally, we plan to extend the MPI parallelism to the energy contour, this will increase the strong scaling capabilities of LSMS, especially for calculations that require many energy point evaluations, such as DMFT, where the number of energy points is increased by O(100) compared to the standard DFT calculations.

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PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN
(Does* not *count toward the 15-page project narrative limit.)

PERSONNEL JUSTIFICATION

The research in this project will be conducted by the PIs as well as postdoctoral researchers who have already been identified or are to be hired. The work in this project falls into three scientific tasks: Magnetic materials, alloys and ferroelectrics and development tasks: Wang-Landau Monte-Carlo development, first principles multiple scattering.

The personnel already in place together with their affiliation and the tasks they will be involved in are:

Dr. Markus Eisenbach, ORNL, Magnetic materials, DMFT development, overall coordination of tasks

Dr. Valentino Cooper, ORNL, High Entropy Oxides

Dr. Mina Yoon, ORNL, Topological quantum materials

Dr. Swarnava Ghosh, ORNL, LSMS development, alloy and quantum material simulations

Dr. Ka Ming Tam, Louisiana State University, Transport and embedding

Dr. Hanna Terletska, Middle Tennesse State University, Typical medium embedding, electron localization, DMFT analysis

Dr. Yang Wang, Pittsburgh Supercomputing Center - Carnegie Melon University, Full Potential Multiple Scattering

Dr. Mariia Karabin, ORNL postdoc supervised by Dr. Eisenbach, LSMS development and Monte-Carlo simulations

Dr. Wasim Mondal, Middle Tennessee State University postdoc supervised by Dr. Terletska, LSMS typical medium embedding, localization

Vishnu Raghuraman Carnegie Mellon University, Graduate Student. Electron conductivity calculations in LSMS

MANAGEMENT PLAN

The work in this project will be performed by a small group of closely collaborating researchers. The PI will coordinate the usage of computational resources and the scientific direction will be jointly by the PIs. We will have regular meetings (with phone in or online participation by the remote collaborators) to monitor the progress of this project in accordance with its milestones. Additionally, the individual tasks have weekly meetings to coordinate the research and development of the respective parts of this project.

The overall project will be lead and coordinated by **Markus Eisenbach**, who is an expert in DFT calculations and statistical physics of magnetic materials and in large scale scientific computing. He will also lead the magnetic materials task and guide the development of the Wang-Landau codes. The alloys task will be lead by **Markus Eisenbach**, the ferroelectric task will be lead by **Valentino R. Cooper** and the functional materials task by **Hanna Terletska** and **Ka Ming Tam** .

Year 1 (2023)			
Milestone	**Details**	**Dates**	**Status (renewals only)**
Defects in HEAs	**Resources:** Summit & Frontier **Node hours:** Summit: 60,000; Frontier: 60,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 0.5 **Software Application:** Quantum Espresso and WL-LSMS **Tasks:** WL-LSMS calculation for MoNbTaWX for $X \in \{\text{Ti, V, Cr, Mn}\}$ to establish ordering phase diagram and database for ML training of surrogate model. Generalized Planar Fault Energy curves for Cantor (Q1-Q2) and refractory (Q3-Q4) alloys as functions of Short Range Order (SRO) and applied stress. **Dependencies:** HEA short range order	Q1-Q4	
Non-magnetic ions in spinel-HEO	**Resources:** Summit & Frontier **Node hours:** Summit: 40,000; Frontier: 30,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** Quantum Espresso & LSMS **Tasks:** Influence of non magnetic ions on the magnetic interactions in spinel-HEOs **Dependencies:** none	Q1-Q2	
Stability and Physical Properties of Delafossite, ABO_2	**Resources:** Summit & Frontier **Node hours:** Summit: 50,000; Frontier: 20,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS + FHI-aims **Tasks:** Combinatorial study of delafossite for their thermodynamic stabilities and physical properties in terms of A and B elements. **Dependencies:** None	Q1-Q4	

Year 1 (2023)			
Milestone	**Details**	**Dates**	**Status (renewals only)**
Skyrmion lattice MnGe	**Resources:** Frontier **Node hours:** 100,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** WL-LSMS **Tasks:** First principles calculation of finite temperature Skyrmions in MnGe **Dependencies:** none	Q4	
Disorder in $MnBi_2Te_4$	**Resources:** Summit & Frontier **Node hours:** Summit: 50,000; Frontier: 20,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS & FHI-aims **Tasks:** Calculation of the magnetic states of $MnBi_2Te_4$ with disorder Monte-Carlo calculations of magnetic transitions **Dependencies:** none	Q2	
LSMS + DMFT development	**Resources:** Summit & Frontier **Node hours:** Summit: 10,000; Frontier: 20,000 **Filesystem storage (TB and dates):** 0.2 **Archival storage (TB and dates):** 0 **Software Application:** LSMS **Tasks:** Implementation and testing of LSMS DMFT+LDA **Dependencies:** none	Q4	
Weyl Semimetal	**Resources:** Summit **Node hours:** 80,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** FHI-aims & LSMS **Tasks:** Magnetic Co vacancies in $Co_3Sn_2S_2$ **Dependencies:** none	Q3	

Year 2 (2024)			
Milestone	**Details**	**Dates**	**Status (renewals only)**
Defects in HEAs	**Resources:** Frontier **Node hours:** 60,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 0.5 **Software Application:** WL-LSMS **Tasks:** LSMS calculation for MoNbTaWXX' for $X, X' \in$ {Ti, V, Cr, Mn} build a database for ML training of surrogate model and Monte-Carlo calculations WL-LSMS simulations of twins and grain boundaries in Cantor and refractory alloys for different cases of SRO. **Dependencies:** Refractory HEA 5-component alloy	Q1-Q4	
spinel - HEO phase diagram	**Resources:** Frontier **Node hours:** 50,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** Quantum Espresso & WL-LSMS **Tasks:** Calculation of the spinel high entropy oxide magnetic phase diagram **Dependencies:** Non-magnetic spinel-HEO	Q1	
LSMS + DMFT for disordered systems	**Resources:** Frontier **Node hours:** 100,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 0 **Software Application:** LSMS **Tasks:** Calculations of LSMS DMFT+LDA incorporating disordered effective medium: $Cu_{1-x}Pd_x$ binary alloys and half-metallic NiMnSb alloys **Dependencies:** LSMS + DMFT development	Q4	

Year 2 (2024)			
Milestone	**Details**	**Dates**	**Status (renewals only)**
Skyrmion lattice MnSi	**Resources:** Frontier **Node hours:** 150,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** WL-LSMS **Tasks:** First principles calculation of finite temperature Skyrmions in MnSi **Dependencies:** none	Q4	
$MnBi_4Te_7$ magnetic phase diagram	**Resources:** Frontier **Node hours:** 20,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS & FHI-aims **Tasks:** Calculation of the magnetic states of $MnBi_4Te_7$ with disorder Monte-Carlo calculations of magnetic transitions **Dependencies:** Disorder in $MnBi_4Te_7$	Q1	
Photovoltaic semiconductors: Silicon	**Resources:** Frontier **Node hours:** 30,000 **Filesystem storage (TB and dates):** 0.1 **Archival storage (TB and dates):** 0.05 **Software Application:** LSMS **Tasks:** Study electron localization in Co-, Ti-, S- doped Si **Dependencies:** none	Q3	
Delafossite with Dopants	**Resources:** Frontier **Node hours:** 50,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS + FHI-aims **Tasks:** Combinatorial study of delafossite for their thermodynamic stabilities and physical properties in terms of A and B elements with dopants. **Dependencies:** Stability and Physical Properties of Delafossite, ABO_2	Q1-Q4	

Year 3 (2025)			
Milestone	**Details**	**Dates**	**Status (renewals only)**
Defects in HEAs	**Resources:** Frontier **Node hours:** 60,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 0.5 **Software Application:** WL-LSMS **Tasks:** WL-LSMS simulations of dislocations in Cantor and refractory alloys for different cases of SRO. **Dependencies:**	Q1-Q4	
Disorder in $MnSb_4Te_7$	**Resources:** Frontier **Node hours:** 20,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS & FHI-aims **Tasks:** Calculation of the magnetic states of $MnSb_4Te_7$ with disorder Monte-Carlo calculations of magnetic transitions **Dependencies:** none	Q2	
Delafossite with Dopants and Disorders	**Resources:** Frontier **Node hours:** 40,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS + FHI-aims **Tasks:** Combinatorial study of delafossite for their thermodynamic stabilities and physical properties in terms of A and B elements with dopants and disorders. **Dependencies:** Delafossite with Dopants and Disorders	Q1-Q4	

Year 3 (2025)			
Milestone	**Details**	**Dates**	**Status (renewals only)**
Application of LSMS+DMFT to disordered systems	**Resources:** Frontier **Node hours:** 200,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS **Tasks:** Calculation of competition between disorder and electron correlation in Si:P and the magnetic semiconductors $Ga_{1-x}Mn_xN$ and $Ga_{1-x}Mn_xAs$. **Dependencies:** LSMS+DMFT for disordered systems	Q4	
Photovoltaic semiconductors: In_2S_3	**Resources:** Frontier **Node hours:** 40,00 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** LSMS & FHI-aims **Tasks:** Study electron localization in V doped In_2S_3 **Dependencies:** none	Q3	
Skyrmions in Ga doped MnSi	**Resources:** Frontier **Node hours:** 200,000 **Filesystem storage (TB and dates):** 0.5 **Archival storage (TB and dates):** 1 **Software Application:** WL-LSMS **Tasks:** Calculation of magnetic interactions in MnSi:Ga Monte-Carlo simulation of pinning and depinning of skyrmions due to disorder **Dependencies:** none	Q4	

PUBLICATIONS RESULTING FROM INCITE AWARDS

(Does* not *count toward the page limit.)

S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D'Azevedo, R. T. Scalettar, T. Pruschke, M. Jarrell, "Parquet approximation for the 4x4 Hubbard cluster", Phys. Rev. E 80, 046706 (2009)

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E. Khatami, K. Mikelsons, D. Galanakis, A. Macridin, J. Moreno, R. T. Scalettar, M. Jarrell, "Quantum Criticality Due to Incipient Phase Separation in the Two-dimensional Hubbard Model", Phys. Rev. B 81, 201101(R) (2010)

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Shu-Xiang Yang, Herbert Fotso, Shi-Quan Su, Dimitrios Galanakis, Ehsan Khatami, Jian-Huang She, Juana Moreno, Jan Zaanen, Mark Jarrell, "Proximity of the Superconducting Dome and the Quantum Critical Point in the Two-Dimensional Hubbard Model", Phys. Rev. Lett. 106, 047004 (2011)

Ka-Ming Tam, H. Fotso, S.-X. Yang, Tae-Woo Lee, J. Moreno, J. Ramanujam, M. Jarrell, "Solving the Parquet Equations for the Hubbard Model beyond Weak Coupling", Phys. Rev. E 87, 013311 (2013)

K.-S. Chen, S. Pathak, S.-X. Yang, S.-Q. Su, D. Galanakis, K. Mikelsons, M. Jarrell, J. Moreno, "Role of the van Hove Singularity in the Quantum Criticality of the Hubbard Model", Phys. Rev. B 84, 245107 (2011)

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M. Eisenbach, C.-G. Zhou, D. M. Nicholson, G. Brown. J. Larkin, T. C. Schulthess. "Thermodynamics of Magnetic Systems from First Principles: WL-LSMS." *CUG 2010 Proceedings* (2010).

G. Brown, A. Rusanu, M. Daene, D.M. Nicholson, M. Eisenbach, and J. Fidlers, "Improved Methods for Calculating Thermodynamic Properties of Magnetic Systems using Wang-Landau Density of States," *J. Appl. Phys.* **109**, 07E161 (2011).

D. M. Nicholson, Kh. Odbadrakh, A. Rusanu, M. Eisenbach, G. Brown, B. M. Evans, III, "First principles approach to the magneto caloric effect: Application to Ni2MnGa", *J. Appl. Phys.* **109**, 07A942 (2011).

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Yang Wang, D. M. C. Nicholson, G. M. Stocks, Aurelian Rusanu, Markus Eisenbach, R. E. Stoller, "A study of radiation damage effects on the magnetic structure of bulk Iron", *J. Appl. Phys.* **109**, 07E120 (2011).

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K. Odbadrakh, A. Rusanu, G. M. Stocks, G. D. Samolyuk, M. Eisenbach, Yang Wang, D. M. Nicholson, "Calculated electronic and magnetic structure of screw dislocations in alpha iron", *J. Appl. Phys.* **109**, 07E159 (2011).

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D. Perera, Y. W. Li, M. Eisenbach, T. Vogel, D. P. Landau "Replica-exchange Wang-Landau sampling: Pushing the limits of Monte Carlo simulations in materials sciences", In *TMS2015 Supplemental Proceedings*, pages 811–818. The Minerals, Metals & Materials Society, John Wiley & Sons, Inc., (2015).

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Xianglin Liu, Jiaxin Zhang, Junqi Yin, Sirui Bi, Markus Eisenbach, Yang Wang, "Monte Carlo simulation of order-disorder transition in refractory high entropy alloys: A data-driven approach", *Computational Material Sciences* **187**, 110135 (2021).

Massimiliano Lupo Pasini, Junqi Yin, Ying Wai Li, Markus Eisenbach, "A scalable algorithm for the optimization of neural network architectures", *Parallel Computing* **104-105**, 102788 (2021).

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Massimiliano Lupo Pasini, Marko Burčul, Samuel Temple Reeve, Markus Eisenbach, Simona Perotto, "Fast and accurate predictions of total energy for solid solution alloys with graph convolutional neural networks", In: "Driving Scientific and Engineering Discoveries Through the Integration of Experiment, Big Data, and Modeling and Simulation. SMC 2021", *Communications in Computer and Information Science* **1512**, 79 (2022).

Mariia Karabin, Wasim Raja Mondal, Andreas Östlin, Wai-Ga D Ho, Vladimir Dobrosavljevic, Ka-Ming Tam, Hanna Terletska, Liviu Chioncel, Yang Wang, Markus Eisenbach, "Ab initio approaches to high-entropy alloys: a comparison of CPA, SQS, and supercell methods", *Journal of Materials Science* (2022).

Curriculum Vitae
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Professional Preparation

University of Bristol, United Kingdom	Ph.D.	2001	Theoretical Physics
Technische Universität Darmstadt, Germany	Dipl. Phys.	1997	Physics
University of Bristol, United Kingdom	B.Sc.	1995	J. Hons. Mathematics & Physics

Appointments

2019-present	Senior R&D Staff, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831
2007-2019	R&D Staff, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831
2006-2007	ORNL Research Scientist, University of Tennessee, Knoxville, TN 37996
2001-2006	Postdoctoral Research Associate, Oak Ridge Associated Universities, Oak Ridge, TN 37831

Five Publications Most Relevant to This Proposal

1. "Monte Carlo simulation of order-disorder transition in refractory High Entropy alloys: a data driven approach", X. Liu, J. Zhang, J. Yin, S. Bi, **M. Eisenbach**, Y. Wang, Computational Material Science 187, 110135 (2021).
2. "Tuning Fermi Levels in Intrinsic Antiferromagnetic Topological Insulators MnBi2Te4 and MnBi4Te7 by Defect Engineering and Chemical Doping", M.-H. Du, J. Yan, V. R. Cooper, **M. Eisenbach**, Advanced Functional Materials, 2006516 (2020).
3. "Predicting the Phase Stability of Multicomponent High-Entropy Compounds", K. C. Pitike, S. KC, **M. Eisenbach**, C. A. Bridges, V. R. Cooper, Chemistry of Materials 32, 7507 (2020).
4. "Deciphering chemical order/disorder and material properties at the single-atom level", Y. Yang, C.-C. Chen, M. C. Scott, C. Ophus, R. Xu, A. Pryor, L. Wu, F. Sun, W. Theis, J. Zhou, **M. Eisenbach**, P. R. C. Kent. R. Sabirianov, H. Zeng, P. Ercius, J. Miao, Nature 542, 75 (2017).
5. "Density-functional Monte-Carlo simulation of CuZn order-disorder transition", S. N. Khan and **M. Eisenbach**, Phys. Rev. B. 93, 024203 (2016).

Research Interests and Expertise

My research is focused on computational approaches to condensed matter physics and material science on an atomistic scale. While my main expertise lies in *ab initio* calculations of magnetic properties of materials and alloys and the development of methods for classical models and classical Monte-Carlo methods. I am one of the main developers of the LSMS electronic structure code. He has authored the original relativistic version of this code and he devised the Wang-Landau LSMS method that combines first principles calculations with classical statistical mechanics to calculate the thermodynamics of magnetic and alloy phase transitions using density functional theory. Additionally, as member of the Scientific Computing group at the NCCS, he provides user liaison for a variety of material science projects ranging from classical simulations

to both DFT and Quantum Monte Carlo based calculation.

Synergistic Activities

- Reviewer: Phys. Rev. Lett., Phys. Rev. B, Phys. Rev E, J. Appl. Phys. IEEE Magnetics
- Awards: ACM 2009 Gordon Bell Prize for Peak Performance, ACM 2008 Gordon Bell Prize for Peak Performance
- Member: American Physical Society, Association for Computing Machinery, Deutsche Physikalische Gesellschaft (Germany)

Collaborators (*past 5 years including name and current institution*)

Gautam Anand (Indian Institute of Engineering Science and Technology, Shibpur, India), Kipton Barros (Los Alamos National Laboratory), Cristian Batista (University of Tennessee, Knoxville), Chien-Chun Chen (National Sun Yat-sen University, Taiwan), S. W. Cheung (Chinese University, Hong Kong), Liviu Chioncel (Universität Augsburg, Germany), Peter Ercius (Lawrence Berkeley National Laboratory), Carlos E. Fiore (Universidade de Sao Paulo, Brazil), Colin L. Freeman (University of Sheffield, United Kingdom), Russel Goodall (University of Sheffield, United Kingdom), Ray Grout (National Renewable Energy Laboratory), Christos Kartsaklis (Apple Inc.), Suffian N. Khan (Microsoft), David P. Landau (University of Georgia, Athens), Ying Wai Li (Los Alamos National Laboratory), Jeff Larkin (NVIDIA Corp.), Justin Lutjens (NVIDIA Corp.), Jianwei Miao (University of California, Los Angeles), Serge M. Nakhmanson (University of Connecticut), Don M. Nicholson (University of North Carolina, Asheville), Kh. Odbadrakh (University of Tennessee, Knoxville), Colin Ophus (Lawrence Berkeley National Laboratory), Dilina Perera (Mississippi State University), Alan Pryor Jr. (University of California, Los Angeles), Steven Rennich (NVIDIA Corp.), Julio C. S. Rocha (Universidade Federal de Minas Gerais, Brazil), Renat F. Sabirianov (University of Nebraska at Omaha), M. C. Scott (Lawrence Berkeley National Laboratory), Fan Sun (University of Buffalo, SUNY), Ka Ming Tam (Louisiana State University, Baton Rouge), Hannah Terletska (Middle Tennessee State University), Wolfgang Theis (University of Birmingham, United Kingdom), Shan-Ho Tsai (University of Georgia, Athens), Thomas Vogel (University of North Georgia), Yang Wang (Pittsburgh Supercomputing Center, Carnegie Mellon University), Li Wu (University of California, Los Angeles), Rui Xu (University of California, Los Angeles), Yongsoo Yang (University of California, Los Angeles), Simuk Yuk (PNNL), Hao Zeng (University of Buffalo, SUNY), Y. Zhao (Chinese University, Hong Kong), Jihan Zhou (University of California, Los Angeles)

Graduate and Postdoctoral Advisors

Graduate Advisors: B. L. Györffy (University of Bristol, UK), J. Kübler (TU Darmstadt, Germany). *Postdoctoral Advisor:* G. M. Stocks (Oak Ridge National Laboratory).

Postdoctoral Advisees

Suffian Khan (Microsoft), Ying Wai Li (LANL), Junqi Yin (ORNL), Zongrui Pei (NETL), Xianglin Liu (Peng Cheng Laboratory, China), Massimiliano Lupo Pasini (ORNL), Jiaxin Zhang (ORNL), Swarnava Ghosh (ORNL), Mariia Karabin (current)

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Professional Preparation:

Vassar College, Poughkeepsie, NY	B.A.	2000	Chemistry
University of Pennsylvania, Philadelphia, PA	Ph.D.	2005	Physical Chemistry
Rutgers University, Piscataway, NJ	Postdoc	2005-2008	Physics

Appointments:

2020 – present	Section Head, Materials Theory, Modeling and Simulations, MSTD, ORNL
2020 – present	Distinguished R&D Staff, Materials Science and Technology Division, ORNL
2019 – 2020	Group Leader, Condensed Matter Theory Group, MSTD,
2017 – present	Associate Editor, Journal of Applied Physics, AIP
2016 – present	Senior R&D Staff, Materials Science and Technology Division, ORNL
2017 – 2019	Team Lead, Materials Theory Group, MSTD, ORNL
2012 - 2016	R&D Staff, Materials Science and Technology Division, ORNL
2008 - 2012	R&D Associate, Materials Science and Technology Division, ORNL

Five Publications Most Relevant to This Proposal (total 123; *h*-index: 35):

K. Pitike, A. Macias, M. Eisenbach, C. A. Bridges, **V. R. Cooper** Computationally accelerated discovery of high entropy pyrochlore oxides *Chem. Mater.* **34** 1459 (2022)

B. Jiang, C. A. Bridges, R. R. Unocic, K. Pitike, **V. R. Cooper**, Y. Zhang, D.-Y. Lin, K. Page Probing the local site disorder and distortion in pyrochlore high-entropy oxides *J. Am. Chem. Soc.* **143**, 4193 (2021)

K. Pitike, S. KC, M. Eisenbach, C. A. Bridges, **V. R. Cooper** Predicting the phase stability of multi-component high entropy compounds *Chem. Mater.* **32**, 7507 (2020)

K. Pitike, A. Marquez-Rossy, A. Flores-Betancourt, D. X. Chen, S. KC, **V. R. Cooper**, and E. Lara-Curzio On the elastic anisotropy of the entropy-stabilized oxide (Mg, Co, Ni, Cu, Zn)O *J. Appl. Phys.* **128**, 015101 (2020)

M. Brahlek, A. R. Mazza, K. Pitike, E. Skoropata, J. Lapano, G. Eres, **V. R. Cooper**, T. Z. Ward Unexpected crystalline homogeneity from the disordered bond network in $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O_3$ films *Phys. Rev. Mater.* **4**, 054407 (2020)

Research Interests and Expertise:

My expertise lies in the field of first principles modeling of novel materials with a focus on electronic structure methods for understanding dispersion interactions and functional materials including piezoelectrics and ferroelectrics.

Honors and Awards:

DOE Early Career Award (2013)
IBM/ACS Graduate Student Award in Computational Chemistry (2002)

Synergistic Activities:

- APS DCOMP (Elected) Member at Large
- ACS Awards Committee
- NSF PIRE Review Panel

- CNMS User Executive Committee, Member at Large
- APS Focus Session: van der Waals Bonding in Advanced Materials co-organizer with Leeor Kronig
- Fundamental Physics of Ferroelectrics and Related Materials Workshop (lead organizer)
- Computational and Data Driven Materials (CDMR5) Review Panel, NSF
- Cyber-Enabled Discovery and Innovation Review Panel, NSF

Mentoring/Outreach Activities:

Summer 2019	ORNL HERE student mentor (N. Meyer, Wake Forest)
Summer 2017	ORNL ASTRO student mentor (K. Pitike, U. Conn.)
Summer 2016	ORNL ASTRO student mentor (K. Pitike, U. Conn. & R. Herchig, U. S. Fl.)
Fall 2014	ORNL HERE sabbatical visitor (K. Donald, Richmond Univ.)
Summer 2014	ORNL HERE student mentor (B. K. Voas, Iowa State)
Summer 2013	ORNL ASTRO student mentor (N. Sivadas, Carnegie Melon)
2013 –2015	Post-doctoral advisor: Dr. Hemant Dixit
Summer 2012	ORNL HERE student mentor (B. K. Voas, Iowa State)
2009 - 2011	Ph. D. visiting student mentor (Dr. Guo Li, Molecular Foundry)

Collaborators:

R. Agarwal (Univ. Puerto Rico, San Juan), D. S. Aidhy (Univ. Wyoming), M. Alexe (Univ. Warwick), S. P. Beckman (Washington State Univ.), K. Berland (Univ. Oslo), I. Bredesen (Univ. Tennessee), P. Canepa (National Univ. Singapore), G. Cao (Univ. Colorado, Boulder), F. Ceballos (Univ. Arkansas), G. Clark (Univ. Washington), K. J. Donald (Univ. Richmond), A. Dzubak (Bowdoin College), T. Ferreira (Formerly ORNL), J. W. Freeland (Argonne), Y. Gao (Shanghai Univ.), Z. Ge (West Virginia Univ.), S. Hong (Korea Institute of Science and Technology), P. Hyldgaard (Chalmers Univ.), Y. Ihm (Pohang Univ. Science and Technology), H. Jeen (Pusan National Univ.), R. S. Katiyar (Univ. Puerto Rico, San Juan), Y. Kim (Sungkyunkwan Univ.), M. Lang (Univ. Tennessee), L. Li (West Virginia Univ.), Q. Li (Shanghai Univ.), Y. Li (Wai), B. Liu (Shanghai Univ.), Y. Liu (Shanghai Univ.), X. Lu (Xidian Univ.), B. I. Lundqvist (Chalmers Univ. retired), T. L. Meyer (Intel), A. Moati (North Carolina State Univ.), J. R. Morris (Ames National Laboratory), S. M. Nakhmanson (Univ. Connecticut), J. Narayan (North Carolina State Univ.), G. D. Nguyen (Univ. British Columbia), J. Nichols (Univ. Arkansas , Little Rock), X. Ou (Chinese Academy of Sciences), T. Pandey (Univ. Antwerp), S. Pantelides (Vanderbilt Univ.), C. Polanco (Formerly ORNL), L. Qiao (Univ. Manchester), S. F. Rus (National Institute for Research and Development in Electrochemistry and Condensed Matter), R. Sachan (Oklahoma State Univ.), Irmak Sargin (Washington State Univ.), E. Schroder (Chalmers Univ.), A. S. Sefat (DOE BES), J. H. Shim (Pohang Univ. Science and Technology), Y. Sharma (Los Alamos National Laboratory), J. Sheng (Renmin Univ. China), H. Sims (Francis Marion Univ.), J. Terzic (Univ. Colorado, Boulder), T. Thonhauser (Wake Forest Univ.), M. Tian (Univ. Tennessee), C. Trautmann (Technische Universitat Darmstadt and GSI Helmholtzzentrum fur Schwerionenforschung GmbH), L. Vlcek (Formerly Univ. Tennessee), P. Wadley (Univ. Nottingham), B. Wang (Shanghai Univ.), H. Xiang (Shanghai Univ.), X. Xu (Univ. Washington), J. Yang (Shanghai Univ.), J. Zhang (Applied Materials), H. Zhao (Univ. Arkansas), H. Zhao (Univ. Colorado, Boulder), H. Zheng (Univ. Colorado, Boulder), Y. Zhou (Shanghai Univ.), S. Philpot (Univ. Florida)

Advisors:

A. Rappe (Univ. Pennsylvania), K. Rabe (Rutgers Univ.)

Former postdoctoral scholars:

Hemant Dixit (BM India), Houlong Zhang (Univ. Arizona), Santosh KC (SJSU), Simuck Yuk (PNNL), Axiel Yaël Birenbaum (NRC Canada), Krishna Pitike (PNNL)

Curriculum Vitae
MINA YOON
myoon@ornl.gov

Professional Preparation

Michigan State University, East Lansing, MI	Ph.D.	2004	Physics
Seoul National University, Seoul, South Korea	M.S.	1999	Physics

Appointments

2021–present Group Leader, Microstructural Evolution Modeling Group, MSTD, Oak Ridge National Laboratory (ORNL)
2021–present Senior R&D Staff Scientist, ORNL
2015–present Joint Professor, Department of Physics and Astronomy, University of Tennessee, Knoxville (UTK)
2009–present R&D staff scientist, ORNL
2008–2011 Max Planck Fellowship, Fritz Haber Institute of the Max Planck Society, Germany
2005–2009 Research Assistant Professor, Department of Physics and Astronomy, UTK
2004–2005 Postdoc, Condensed Matter Physics, ORNL

Five Publications Most Relevant to This Proposal (total 105; h-index:41)

- Cobalt-Based Magnetic Weyl Semimetals with High-Thermodynamic Stabilities, W. Luo, Y. Nakamura, J. Park, and **M. Yoon**, *njp Comp. Mat.* **7**, 1 (2021).
- Quantum Phase Engineering of Two-Dimensional Post-Transition Metals by Substrates: Toward a High-Temperature Quantum Anomalous Hall Insulator, L. Zhang, C. Park, and **M. Yoon**, *Nano Lett.* **20** (10), 7186–7192 (2020).
- GPU-Aceleration of the ELPA2 Distributed Eigensolver for Dense Symmetric and Hermitian Eigenproblems, V. W.-z. Yu, J. Moussa, P. Kus, An. Marek, P. Messmer, **M. Yoon**, H. Lederer, V. Blum, *Comp. Phys. Comm.* **262**, 107808 (2020).
- GPGPU-Accelerated Large-Scale Electronic Structure Theory with a First-Principles All-Electron Code, W. P. Huhn, B. Lange, V. W.-z. Yu, **M. Yoon**, V. Blum, *Comp. Phys. Commun*. **254**, 107314 (2020).
- First-Principles Prediction of New Electrides with Nontrivial Band Topology Based on One-Dimensional Building Blocks, Changwon Park, Sung Wng Kim, **Mina Yoon**, *Phys. Rev. Lett.* **120**, 26401 (2018).

Research Interests and Expertise

Dr. Mina Yoon is an expert in computational materials science and theoretical condensed matter physics. In this project she will investigate the properties of novel topological quantum materials and the impact of defects and disorders. She will use FHI-aims code, an all-electron DFT code, where she implemented a van der Waals density functional scheme, also led a project to GPU accelerate the code, and developed a hybrid scheme for global structure optimization. Recently she also developed a computational materials platform that led to the discovery of the first nontrivial quantum electride. Those schemes will be utilized in this project.

Honors and Awards:

- 2021 ORNL Innovation Award
- R&D 100 Award (2021) UCC: Ultraconductive Copper-Carbon Nanotube Composite
- Outstanding Scholarly Output team award in the Science and Technology category in 2020 UT-Battelle Awards Night program, September 2020.
- The Lee Hsun Young Scientist Award from the Institute of Metal Research, Chinese Academy of Science, October 2017.

- Max Planck Fellowship, Fritz Haber Institute of the Max Planck Society, Germany, 2008-2011.

Synergistic Activities

- Secretary-Elect of the Electronics Division of the American Ceramic Society, since 2022.
- Editorial Board – Carbon (since 2020); Journal of Theoretical Chemistry (2012-2017); The Scientific Pages of Atoms and Molecules (since 2017); The journal of Chemistry: Theoretical Chemistry (since 2017); Annals of Atoms and Molecules (since 2017); International Journal of Molecular Sciences (IF:4.556, since April 2021); Materials (IF:3.057, since April 2021).
- Organizing conferences

  Outreach chair (Organizing Committee), World Outreach Workshop: Focus on 5G and Beyond, sponsored by the American Ceramics Society, July 7, 2021; Organizer of a symposium on "Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics" at the Electronic Materials Applications (EMA) conference, sponsored by the American Ceramic Society, EMA, since 2014; Organizer of a symposium on "From Basic Science to Agile Design of Functional Materials: Aligned Computational and Experimental approaches and Materials Informatics" at the Electronic Materials Applications (EMA) conference, sponsored by the American Ceramic Society, EMA 2020, Florida, Jan 21-24, 2020; Organizer 2019; Co-organizer of DMF Focus topics at the APS March meeting, L.A., March 2018; Organizer, "Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches" at the EMA conference, sponsored by the American Ceramics Society, Orlando, Florida, January 2018; Co-organizer of a symposium on "Recent Advances in Computer-aided Materials Design" at Materials Science & Technology 2017, Oct. 8-12, 2017, Pittsburgh PA; Organizer, CECAM Workshop on First Principles Theory and Modeling in Organic Electronics, Lausanne, Switzerland (2011); Organizer, CECAM Symposium at Psi-k 2010 on Organic Electronics for Energy Research, Berlin, Germany (2010).
- Committee/Chair

  Committee of Computational resources, Quantum Science Center, since September 2020.; Committee of CNMS Awards, September 2020; Committee of Quantum Materials over Coffee, seminar series at ORNL (since July 2020); Ph.D thesis committee/advisor of Jinseon Park, UTK, 2016-2020; Session chair at American Physical Society March meetings, 2006-2008, 2015-2018; Organization committee of Advance Materials Congress 2017-2018; Guiding technical program on APS March meeting 2018; Ph.D thesis committee of Chandani Nandadasa, Mississippi State University, 2018; Session Chair at the Synthesis and Processing Science Principle Investigators (DOE-BES programs) Meeting, Nov. 2015; Organization Committee, Conference on Computational Physics 2011, Gatlinburg, Tennessee, 2011.

Collaborators (*past 5 years including name and current institution*)

Chan, Maria (Argonne National Lab); Huhn, William (Argonne National Lab); Mahjouri-Samani, Madoud (Auburn U.); Smith, Sean (Australian National U.); Huang, Bing (Beijing CSRC); Wei, Su-Huai (Beijing CSRC); Blum, Volker (Duke U.); Kumar Satish (Georgia Tech); Tian, Mengkun (Georgia Tech.); Park, Changwon (IBS, Korea); Kim, Yong-Hyun (KAIST, Korea); Kim, Yong-Sung (KRISS, Korea); Carbogno, Christian (FHI, Germany); Luca, Ghiringhelli (FHI, Germany); Scheffler, Matthias (FHI, Germany); Zhang, Pengpeng (Michigan State U.); Hu, Zhili (Nanjing U, China); Brown, Craig (NIST); Bernholc, Jerzy (North Carolina State U.); Lu, Wenchang (North Carolina State U.); Lee, Jaekwang (Pusan National U., Korea); Yacobson, Boris (Rice U.); Sung Wng Kim (Seungkyunkwan U., Korea); Mavrokefalos, Anastassios (U. Houston); Liu, Feng (U. Utah); Choi, Joshua (U. Virginia); Lee, Seung-Hun (U. Virginia); Duscher, Gerd (U. Tennessee); Gu, Gong (U. Tennessee); Zhang, Lizhi (U. Tennessee), Ghosh, Avik (U. Virginia), Hu, Xiao (U. Virginia); Zhang, Depei (U. Virginia)

Curriculum Vitae

Swarnava Ghosh
Computational Scientist
National Center for Computational Sciences
Oak Ridge National Laboratory
1 Bethel Valley Road
Oak Ridge, TN 37831
ghoshs@ornl.gov

Professional Preparation

Georgia Institute of Technology, Atlanta, USA	Ph.D.	2016	Civil Engineering
Georgia Institute of Technology, Atlanta, USA	M.S.	2015	Civil Engineering
Jadavpur University, Kolkata, India	B.S.	2012	Construction Engineering

Appointments

2022 - Present: Computational Scientist, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831
2020 – 2022: OLCF Distinguished Postdoctoral Research Associate, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831.
2016-2020: Postdoctoral Research Associate, Department of Mechanical and Civil Engineering, California Institute of Technology, Pasadena, CA 91125.
2012-2016: Graduate Research & Teaching Assistant: School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, GA 30332.

Five Publications Most Relevant to This Proposal

1. Swarnava Ghosh and Kaushik Bhattacharya, "Spectral quadrature for the first principles study of crystal defects: Application to magnesium", Journal of Computational Physics, Volume 456, May 2022, 111035.
2. Ying Shi Teh, Swarnava Ghosh and Kaushik Bhattacharya, "Machine-learned prediction of the electronic fields in a crystal", Mechanics of Materials, Volume 163, December 2021, 104070.
3. Swarnava Ghosh and Phanish Suryanarayana, "Electronic structure study regarding the influence of macroscopic deformations on the vacancy formation energy in aluminum", Mechanics Research Communications, 99 (2019) 58-63
4. Swarnava Ghosh and Phanish Suryanarayana, "SPARC: Accurate and efficient finite-difference formulation and parallel implementation of Density Functional Theory: Extended systems", Computer Physics Communications, 216 (2017) 109-125
5. Swarnava Ghosh and Phanish Suryanarayana, "SPARC: Accurate and efficient finite-difference formulation and parallel implementation of Density Functional Theory: Isolated clusters", Computer Physics Communications, 212 (2017) 189-204

Research Interests and Expertise

Broadly in the area of materials, computational physics and scientific computing with emphasis on development of theoretical and computational methods, integrating recent advances in applied physics, mathematics and computational science to model behavior of materials and structures across length and time scales over a diverse range of conditions. Focus on large scale first

principles simulations of materials using methods such as Kohn-Sham Density Functional Theory.

Synergistic Activities

- Co-organizer with Mauricio Ponga, Jaime Marian, Dennis Kochmann of mini-symposium on "Recent Advances in Modeling and Simulation Nano- and Micromechanics of Materials" at SES Annual Technical Meeting 2022.
- Co-organizer with Phanish Suryanarayana and Amartya Banerjee of mini-symposium on "Theory and Simulation of Nanomaterials" at SES Annual Technical Meeting 2019, "First Principles Simulations and their applications to the Mechanics of Materials" at SES Annual Technical Meeting 2020.
- Reviewer for Journal of Computational Physics, Journal of Applied Physics, Mathematics, Computation, Applied Sciences.
- Judge for Aeronautics and Mechanical Engineering presentation session at Summer Undergraduate Research Fellow (SURF) Seminar, Fall 2017 and Fall 2019 at California Institute of Technology.
- Membership of Materials Research Society, Society for Industrial and Applied Mathematics, Society of Engineering Science

Collaborators (past 5 years)
Mauricio Ponga (University of British Columbia, Canada)
Gautam Anand (Indian Institute of Engineering Science and Technology, Shibpur, India)
Ka Ming Tam (Louisiana State University, Baton Rouge)
Hannah Terletska (Middle Tennessee State University)
Yang Wang (Pittsburgh Supercomputing Center, Carnegie Mellon University)
Markus Eisenbach (Oak Ridge National Laboratory)
Kaushik Bhattacharya (California Institute of Technology)
Phanish Suryanarayana (Georgia Institute of Technology)
Amartya Banerjee (University of California Los Angeles)
Ying Shi Teh (Lawrence Livermore National Laboratory)

Graduate and Postdoctoral Advisors

Graduate Advisor: Phanish Suryanarayana (Georgia Institute of Technology)

Postdoctoral Advisors: Markus Eisenbach (Oak Ridge National Laboratory), Kaushik Bhattacharya (California Institute of Technology)

Curriculum Vitae
Ka Ming Tam
Department of Physics and Astronomy, Louisiana State University,
202 Nicholson Hall, Baton Rouge, Louisiana 70803
kmtam@lsu.edu
http://tamkaming.com/cms/
225-578-4718

Professional Preparation

Boston University, Boston, MA, USA	Ph.D.	2008	Physics
The Chinese University of Hong Kong, Hong Kong, China	M.Phil.	2002	Physics
The Chinese University of Hong Kong, Hong Kong, China	B.S.	2000	Physics

Appointments

2019 – present	Research Assistant Professor Department of Physics and Astronomy, Louisiana State University
2010 – 2019	Research Associate Department of Physics and Astronomy, Louisiana State University
2007 – 2010	Postdoctoral Researcher Department of Physics and Astronomy, University of Waterloo, Canada

Five Publications Most Relevant to This Proposal

Herbert Fotso, Ka-Ming Tam, and Juana Moreno ``Beyond quantum cluster theories: multiscale approaches for strongly correlated systems'', *Quantum Sci. Technol. 7*, 033001 (2022).

Ka-Ming Tam, Herbert Fotso, S.-X. Yang, Tae-Woo Lee, Juana Moreno, J. Ramanujam, and Mark Jarrell, ``Solving the parquet equations for the Hubbard model beyond weak coupling'', Phys. Rev. E 87, 013311 (2013).

Chinedu Ekuma, Hanna Terletska, Ka-Ming Tam, Zi-Yang Meng, Juana Moreno, and Mark Jarrell, ``Typical Medium Dynamical Cluster Approximation for the study of Anderson Localization in Three Dimensions", Phys. Rev. B 89, 081107 (2014).

Ka-Ming Tam, Hanna Terletska, Tom Berlijn, Liviu Chioncel, and Juana Moreno, ``Real Space Quantum Cluster Formulation for the Typical Medium Theory of Anderson Localization'', *Crystals 11(11)*, 1282 (2021).

Ka-Ming Tam, Yi Zhang, Hanna Terletska, Yang Wang, Markus Eisenbach, Liviu Chioncel, and Juana Moreno, ``Application of the locally self-consistent embedding approach to the Anderson model with non-uniform random distributions'', Ann. Phys. (N.Y.) 168480 (2021).

Research Interest and Expertise

Dynamical Mean Field Theory--Applying dynamical mean field approximation and its generalization dynamical cluster approximation with quantum Monte Carlo solver for cuprates and heavy fermion compounds.

Parquet Formalism and Functional Renormalization Group--Development of self-consistent parquet formalism which sums the parquet diagrams into infinite order and non self-consistent functional renormalization group method for strongly correlated systems.

Disordered and Frustrated Classical and Quantum Systems--Developing and applying large scale Monte Carlo simulations for random frustrated systems both at the classical and quantum levels. Including GPU multispin bit-level coding.

Machine Learning Approach for Materials Science--Applying machine learning methods for identifying order parameters and detecting phase transition.

Synergistic Activities
Journal Referee for: Physical Review Letters, Physical Review B, Physical Review E, and Scientific Report
Conference Session Chair for: APS Macrh Meeting 2015, Session Q24: Focus Session: Quantum Monte Carlo Simulations of Fermion and Boson Systems II

Collaborators (past 5 years)
Juana Moreno, Louisiana State University
Yi Zhang, University of Chinese Academy of Sciences
Kalani Hettiarachchilage, The College of New Jersey
Hanna Terletska, Middle Tennessee State University
Wei Ku, Shanghai Jiao Tong University
Enzhi Li, Amazon
Peng Zhang, Xi'an Jiaotong University
Chinedu Ekuma, Lehigh University
Tom Berlijn, Oak Ridge National Laboratory
Sheng Feng, Microsoft
Ye Fang, Louisiana State University
Zhifeng Yun, ARM
J. Ramanujam, Louisiana State University
Nicholas Walker, Lawrence Berkeley National Laboratory
Samuel Kellar, L3Harris
Liviu Chioncel, University of Augsburg
David Campbell, Boston University
Nahom Yirga, Boston University
Herbert Fotso, SUNY Albany
Eric Dohner, SUNY Albany
Nathaniel Wrobel, Louisiana State University
Anshumitra Baul, Louisiana State University
Chakradhar Rangi, Louisiana State University
Mariia Karabin, Oak Ridge National Laboratory
Wasim Mondal, Middle Tennessee University
Andreas Ostlin, University of Augsburg
Wai-Ga Ho, Florida State University
Vladimir Dobrosavljevic, Florida State University
Yang Wang, University of Pittsburgh
Markus Eisenbach, Oak Ridge National Laboratory
Andreas Weh, University of Augsburg
Daniel Bauernfeind, Flatiron Institute
Hans Gerd Evertz, Graz University of Technology
Krzysztof Byczuk, University of Warsaw
Dieter Vollhardt, University of Augsburg

Curriculum Vitae
HANNA TERLETSKA
Department of Physics and Astronomy
Middle Tennessee State University
Box 71, 1301 East Main Street, Murfreesboro, TN 37132
Phone: 615-898-2792
Email: Hanna.Terletska@mtsu.edu

Professional preparation

Drohobych State Ivan Franko University, Ukraine	Physics	B.S.	2003
Florida State University	Physics	Ph. D.	2011
Brookhaven National Laboratory	Cond. Matter Theory	Postdoc	2011-2013
Louisiana State University	Comp. Cond. Matter	Postdoc	2013-2015
Ames Laboratory	Material Science	Postdoc	2015-2016
University of Michigan	Comp. Cond. Matter	Postdoc	2016-2017

Appointments

08/01/ 2017- ongoing, Assistant Professor, Middle Tennessee State University, Murfreesboro, TN

Five publications most closely related to the proposed project

1. M. Karabin, W. Mondal, A. Ostlin, W.G. Ho, v. Dobrosavljevic, K.M. Tam, H. Terletska, L. Chioncel, Y. Wang, M. Einserbach, "Ab initio Approaches to High Entropy Alloys: A Comparison of CPA, SQS, and Supercell Methods", J Mater Sci (2022).
2. H. Terletska, Y. Zhang, K. M. Tam, T. Berlijn, N. S. Vidhyadhiraja, M. Jarrell, "Review: Systematic quantum cluster typical medium method for the study of localization in strongly disordered electronic systems", App. Sci., 8(12) (2018).
3. A. Ostlin, Y. Zhang, H. Terletska, F. Beiu, V, Popescu, K. Byczuk, L. Vitos, M. Jarrell, D. Vollhardt, L. Chioncel, "Ab initio typical medium theory of substitutional disorder", Phys. Rev. B, 101(1), 014210 (2020).
4. H. Terletska, A. Moilanen, Y. Zhang, K. Tam, N. S. Vidhyadhiraja, Y. Wang, M. Eisenbach, L. Chioncel, J. Moreno, "Non-local corrections to the typical medium theory of Anderson localization", Annals of Physics, 168454 (2021).
5. Y. Zhang, R. Nelson, K. -M. Tam, W. Ku, U. Yu, N. S. Vidhyadhiraja, H. Terletska, J. Moreno, M. Jarrell, T. Berlijn, "Origin of localization in Ti-doped Si". Phys. Rev. B, 98(17), 174204 (2018).

Research Interests and Expertise

- Disordered systems and Anderson localization.
- Strongly correlated electrons.
- Quantum criticality; metal-insulator transitions; topological insulators; charge order.

Synergistic Activities

- MTSU Advisory Research Board invited member.

- Grants reviewer for: NSF CAREER, NSF OAC, NSF DMR, NSF GRFP programs, DOE and DOE Early Career, Austrian Science Fund, Oak Ridge Nat. Lab CNMS user proposals, NSF/XSEDE allocation review committee.
- Reviewer for Nature Physics, Phys. Rev. Lett., Phys. Rev. B; and for Computer Physics Communications journal, Physica B, Journal of Electronic Materials.
- Faculty advisor for Women in Physics group, MTSU (2018-present). Advisory board member of MTSU Women in STEM.
- Computational Workshop co-organizer: "A toolkit for Order-N first-principles study of the electronic metal-insulator transition", Louisiana State University, 2019; "Numerical methods for studying electron localization in Quantum materials", LSU 2020, 2021.

Collaborators:
Thomas Maier, Oak Ridge National Laboratory, Tom Berlijn, Oak Ridge National Laboratory, Markus Eisenbach, Oak Ridge National Laboratory, Emanuel Gull, University of Michigan, Yang Wang, Pittsburg Supercomputing Center, N. S. Vidhyadhiraja, Jawaharlal Nehru Centre for Advanced Scientific Researc, India, Yi Zhang, Institute of Physics Chinese Academy of Sciences, Ka Ming Tam, Louisiana State University, Sergei Iskakov, University of Michigan, Joseph Paki, Michigan Tech Research Institute, Tianran Chen, West Chester University, Liviu Chioncel, University of Augsburg, Dieter Vollhardt, University of Augsburg, Juana Moreno (Louisiana State University), Vladimir Dobrosavljevic (Florida State University).

Curriculum Vitae

Yang Wang

Pittsburgh Supercomputing Center, Carnegie Mellon University | ywg@psc.edu | 412-268-2795 (O)

Professional Preparation

1982	**B.S.**, Theoretical Physics, Department of Modern Physics, University of Science and Technology of China
1985	**M.E.**, Electron Physics, Institute of Electronics, Chinese Academy of Sciences
1993	**Ph.D.**, Physics, Department of Physics, Florida Atlantic University
1993 - 1996	**Postdoctoral Researcher**, Metals and Ceramic Division, Oak Ridge National Laboratory

Appointments

1996 - present	**Senior Computational Scientist,** Pittsburgh Supercomputing Center, Carnegie Mellon University, Pittsburgh, PA
2010 - present	**Adjunct Faculty,** Department of Physics, Duquesne University, Pittsburgh, PA Teaching advanced physics courses.
1993 - 1996	**Postdoctoral Researcher,** Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN

Five Publications Most Relevant to This Proposal

- Karabin, M., Mondal, W.R., Östlin, A. Wai-Ga D. Ho, Vladimir Dobrosavljevic, Ka-Ming Tam, Hanna Terletska, Liviu Chioncel, Yang Wang & Markus Eisenbach, "Ab initio approaches to high-entropy alloys: a comparison of CPA, SQS, and supercell methods." J Mater Sci (2022). https://doi.org/10.1007/s10853-022-07186-9
- Vishnu Raghuraman, Yang Wang, and Michael Widom, "An investigation of high entropy alloy conductivity using first-principles calculations," Appl. Phys. Lett. **119**, 121903 (2021). https://doi.org/10.1063/5.0065239
- J.S. Faulkner, G.M. Stocks, and Yang Wang, "Multiple Scattering Theory: Electronic Structure of Solids" IOP Publishing Ltd 2018, ISBN:978-0-7503-1488-6.
- Yi Zhang, Hanna Terletska, Ka-Ming Tam, Yang Wang, Markus Eisenbach, Liviu Chioncel, and Mark Jarrell, "Locally self-consistent embedding approach for disordered electronic systems," Phys. Rev B **100**, 054205 (2019).
- Yang Wang, G.M. Stocks, W.A. Shelton, D.M.C. Nicholson, W.M. Temmerman, and Z. Szotek, "Order-N Multiple Scattering Approach to Electronic Structure Calculations", Phys. Rev. Lett., **75**, 2867 (1995)

Research Interests and Expertise

Primary research interests include computational condensed matter physics and materials science. Research expertise includes multiple scattering theory and high performance Green function based ab initio methods for the study of random alloys.

Synergistic Activities

- Served as a Ph.D. committee member for several graduate students from the Physics Department of Carnegie Mellon University, and advised undergraduate and graduate students on their research in computational physics
- Served as referee for NSF/XSEDE Allocation Review Committee, and referee for scientific journals, including Physical Review B, Physical Review Letter, Journal of Physics: Condensed Matter, Computer Physics Communications, etc.
- Received Gordon-Bell Prize for best achievement in high-performance computing
- The work on developing and implementing a linear scaling ab initio electronic structure calculation method has been included in Year 2000 Permanent Research Collection on Information Technology at the Smithsonian's National Museum of American History

Collaborators

Dayal, Kaushik	Carnegie Mellon University
Dobrosavljevic, Vladimir	Florida State University
Eisenbach, Markus	Oak Ridge National Laboratory
Faulkner, J. Sam	Florida Atlantic University
Kumta, Prashant	University of Pittsburgh
Stocks, G. Malcolm	Oak Ridge National Laboratory
Tam, Ka-Ming	Louisiana State University
Terletska, Hanna	Middle Tennessee State University
Velikokhatnyi, Oleg	University of Pittsburgh
Widom, Mike	Carnegie Mellon University
Zhang, Xiaoguang	University of Florida
Zhang, Yi	Kavli Institute for Theoretical Sciences in Beijing

Section 6: Software Applications and Packages

Question #1

Please list any software packages used by the project, and indicate if they are on open source or export controlled.

Application Packages

Package Name

LSMS/MuST

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

FHI-aims

Indicate whether Open Source or Export Controlled.

Export Controlled

Package Name

Quantum Espresso

Indicate whether Open Source or Export Controlled.

Open Source

Section 7: Wrap-Up Questions

Question #1

National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information

obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.

The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.

Proprietary Information

Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?

Yes

Will the proposed project use proprietary information, intellectual property, or licensing?

No

Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?

If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.

No

Question #2

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.

PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.

Export Control

Does this project use or generate sensitive or restricted information?

No

Does the proposed project involve any of the following areas?

i. Military, space craft, satellites, missiles, and associated hardware, software or technical data

ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data

iii. Encryption above 128 bit software (source and object code)

iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)

No

Does the proposed project involve International Traffic in Arms Regulations (ITAR)?

No

Question #3

The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.

Health Data

Will this project use health data?

No

Will this project use human health data?

No

Will this project use Protected Health Information (PHI)?

No

Question #4

The PI and designated Project Manager agree to the following:

Monitor Agreement

I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.

Yes

I agree to provide periodic updates of research accomplishments and to acknowledge INCITE and the LCF in publications resulting from an INCITE award.

Yes

I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.

Yes

I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.

Yes

Section 8: Outreach and Suggested Reviewers

Question #1

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Outreach

Question #2

Suggested Reviewers

Section 9: Testbed Resources

Question #1

The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)

The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation.

The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: https://www.alcf.anl.gov/alcf-ai-testbed.

Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.

Document3.pdf
The attachment is on the following page.

No testbed resources are requested.