Application Title: High-throughput Autonomous Materials Discovery for Extreme Conditions (HAMDEC) at TAMU

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Key Participating Units: COE, COAS
RDF Amount Requested ($): $1,495,394.45

Executive Summary

We aim to develop an autonomous, high throughput (HTP) materials discovery framework to explore complex materials design spaces in an accelerated manner. More specifically, our objective is to lay the foundation for an **Autonomous Robotic Materials Scientist (ARMS)**, an automated and modular materials synthesis, characterization, testing and simulation facility. ARMS is central to our efforts to create an AI-driven platform capable of exponentially accelerating the entire materials discovery cycle. ARMS will consist of the HAMDEC physical facility as well as an interface to High Performance Research Computing (HPRC) resources to achieve autonomy through an AI-enabled 'brain'. The proposed HAMDEC facility will be coupled with the current work on developing a highly transferrable and application- and materials-agnostic data driven computational framework for accelerated materials discovery and development. Specifically, we seek to exploit our recently developed BIRDSHOT (Batch-wise Improvement in Reduced Materials Design Space using a Holistic Optimization Technique) framework, which is capable of seamlessly integrating multi-scale simulations, advanced synthesis and characterization workflows as well as physics-informed machine learning (ML) within a Bayesian AI fabric capable of 'learning' materials spaces in an iterative manner. With funding by ARPA-E, DOD, NASA and NSF, we have already demonstrated the feasibility of BIRDSHOT as an algorithmic approach to materials discovery. However, BIRDSHOT so far has been deployed through highly distributed, human-driven traditional synthesis, characterization, and simulation operations. The automated and integrated nature of HAMDEC will provide us with the means to demonstrate that BIRDSHOT can autonomously drive highly complex discovery workflows with minimal human intervention. Our **long-term vision** is to establish a one-of-a-kind network of robotic platforms, launching a dust-to-product foundry at TAMU, where scientists within the broader TAMU community and beyond can design, deploy and test on-demand autonomous materials discovery tasks. We intend for this platform to be the seed of a national facility dedicated to realizing the *materials science laboratories of the future*.

A key barrier to realize this vision is the lack of a fully automated materials synthesis, processing, and characterization workflow. As a first step, we are seeking to acquire and integrate different modules of the ARMS platform, which will initially include a multi-material (up to 16 different materials) bulk metal directed energy deposition system equipped with an automated powder feeding system; a fully automated thermo-mechanical processing platform; an automated metallographic sample preparation station, and an automated system to measure the materials' mechanical properties. This initial set up will be augmented through the addition of other modules, such as a fully automated mechanical and fatigue tester, and automated thermal, electrical, microstructural, and magnetic property measurement systems. Eventually, all the modules will be integrated using dedicated robotic sample manipulation systems, minimizing human intervention throughput the entire workflow. In the medium to long term, we envision full integration with HPRC resources not only to control the process but also to aid in the characterization as well as the on-demand simulation of the materials being explored. ARMS will support COE and COAS research funded by federal agencies as well as collaborative projects involving industrial partners across the nation—the leading technology companies in the US recognize autonomous materials platforms as a key strategic enabler for faster product development. Specifically, the RDF will be instrumental to make a strong case for the MRI, the NSF mid-scale infrastructure and will help TAMU compete for an upcoming NASA-STRI and Army Center proposal. Finally, HAMDEC will be leveraged to attract top faculty in the general area of autonomous science, including two CRI/GURI candidates. The requested instruments will be placed in Materials Development and Characterization Center (MDC^2), a sustainable, self-supported user facility with four full-time research scientists and with existing support infrastructure.