Application Title: **High-Throughput Automated Materials Discovery Platform at TAMU**

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Key Participating Units: COE, COAS
RDF Amount Requested ($): $1,450,000

Executive Summary

The discovery of new materials is crucial for sustainable energy, transportation, healthcare, infrastructure, and defense advancements. However, despite progress in high throughput (HTP) computational tools, the experimental validation and scale-up of materials development, particularly in synthesis, processing, characterization, and testing of bulk alloys, remains challenging. The notion of autonomous research platforms offers a new paradigm for scientific discovery. Still, significant challenges remain, particularly in developing automated/autonomous materials discovery workflows that integrate synthesis, processing, characterization, and testing at bulk scales.

To address this challenge, we will establish an **Automated Robotic Materials Scientist (ARMS)** platform at TAMU, a modular alloy design, synthesis, processing, characterization, and testing platform as an integrated "*Dust-To-Product Alloy Foundry*" modeled after semiconductor foundries and capable of operating under different modalities within a novel "alloy-discovery-as-a-service" paradigm. We propose to design ARMS with a modular architecture that will eventually combine multi-material additive manufacturing (AM)-based synthesis, hybrid thermomechanical processing and sample preparation, multi-scale testing and characterization modules, and autonomous robotic arm and robotic translational stages for module integration and sample transfer. The experimental platform will be integrated into the High-Performance Research Computing (HPRC) cyberinfrastructure, enabling the *in-silico* synthesis of the alloys' digital twins and managing the flow of experimental data generated during ARMS' operation. Our **long-term vision** is to establish, through the launch of ARMS, a one-of-a-kind network of robotic platforms where scientists within the broader TAMU community and beyond can design, deploy, and test on-demand materials discovery tasks. We intend this platform to be the seed of a national facility dedicated to realizing the ***materials laboratories of the future***.

To demonstrate the concept and compete for large-scale external funding, we are seeking to acquire key modules of the ARMS platform (a multi-material, bulk sample, directed energy deposition system; a fully automated thermo-mechanical processing system; an automated sample preparation station, and an automated system to measure mechanical properties of materials) and integrate them with the existing modules. To ensure convenient access for the TAMU and external research community, ARMS will be housed at the Materials Development and Characterization Center (MDC^2), which is a fully accessible user facility utilized by over 60 distinct PIs from 3 different colleges, 16 departments, industry, and other universities, strategically located between the COE and COAS quarters. For further expansion of the ARMS platform, we will seek funding from NSF-MRI, the NSF mid-scale infrastructure grants (R1 and R2), and DOD DURIP programs. **This initial setup will also help TAMU compete better for an NSF AI Institute-Materials call. In fact, the PI and the Co-PIs of this RDF proposal were selected as the PI and the Co-PIs of the NSF-AI Institute proposal from TAMU.** In addition, ARMS will directly support existing programs at TAMU, such as ARPA-E (ULTIMATE and GAMOW, $3.5M), DOE-EFRC (REMIND-$10M), NSF-DMREF ($2M), NSF-FM ($3M), ARL, NASA, and AFRL. The PIs have successfully demonstrated the integration of human-led (slow) material synthesis and characterization workflows with simulations and physics-informed machine learning (ML) in some of these programs. As a testament to our national leadership, the Army Research Laboratory has recently selected TAMU to host the High-Throughput Materials Discovery for Extreme Environments Center (HTMDEC-$10M, 8 PIs from 3 departments). ARMS will directly support the HTMDEC Center. ARMS will emerge as the cornerstone of a future national facility, leading a transformative design-driven autonomous approach to alloy development characterized by unprecedented speed and efficiency. The user base for this platform will include 29 faculty in 2 colleges and 11 departments.