Batch-wise Improvement in Reduced Design Space using a Holistic Optimization Technique (BIRDSHOT)

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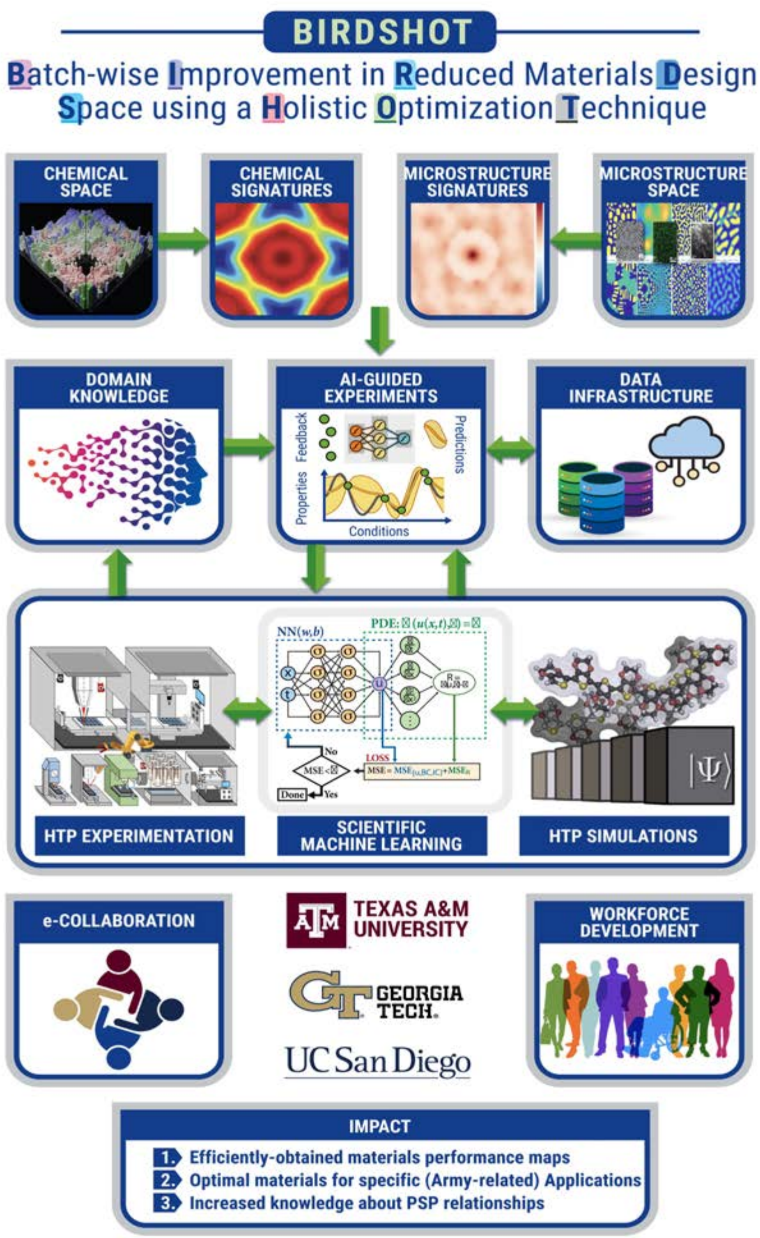
BIRDSHOT



Our **vision** is to develop an application- and materials-agnostic framework for the accelerated discovery of Army relevant-materials and materials systems.

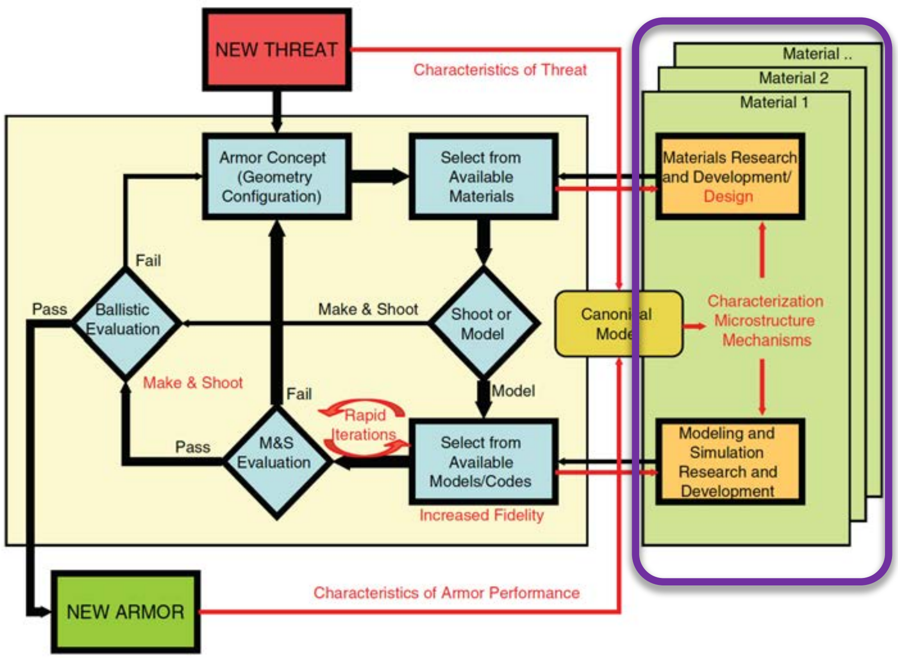
Our **mission** is to deploy integrated experimental-computational-Artificial Intelligence (AI)/Machine Learning (ML) platform for the accelerated discovery of advanced structural materials for Warfighter-relevant applications

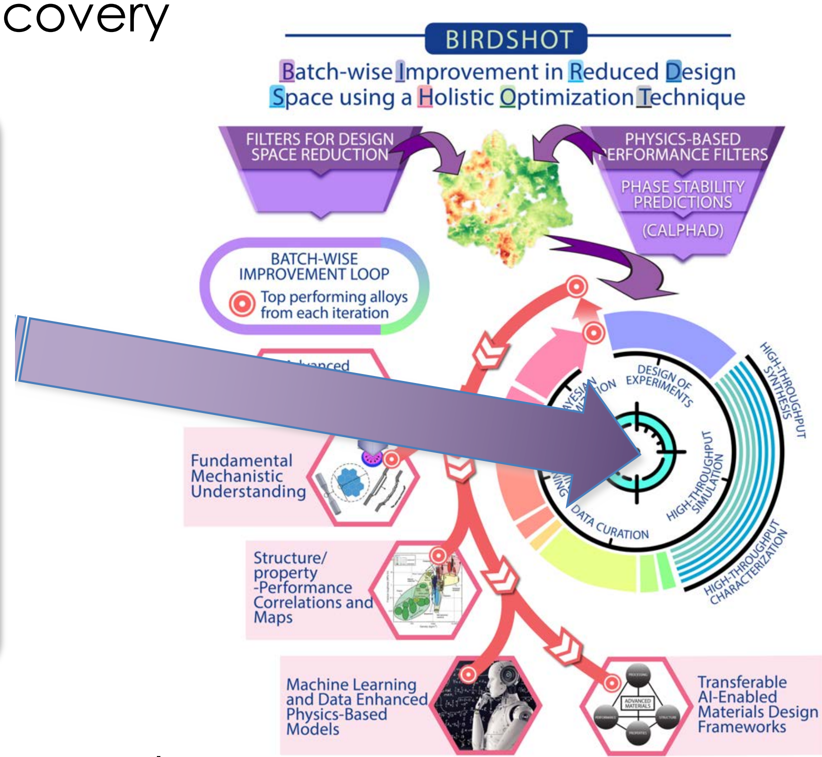
BRDSHOT LEADS

- Raymundo Arróyave, TAMU, (Alloy Design, Bayesian Materials Discovery)
- George Pharr (NAE), TAMU (High Strain Rate Deformation, HSR, HTP Nano-Indentation)
- Ned Thomas (NAE), TAMU (High Strain Rate Deformation, HSR, HTP LIPIT)
- Surya Kalidindi, GTech, (Data-Driven Materials Design, ML+Physics Models for Materials Behavior)
- Ken Vecchio, UCSD, (High-throughput Materials Synthesis)
- Ibrahim Karaman, TAMU (Microstructure-Sensitive Materials Design, HTP Materials Synthesis)
- Dimitris Lagoudas, TAMU, (Mechanics of Materials)
- Ankit Srivastava, TAMU (Microstructure Mechanics, HSR Deformation Simulations, Bayesian Materials Discovery)
- Others: Douglas Allaire, TAMU (Multi-Disciplinary Systems Design and Optimization)

BIRDSHOT's VISION

Accelerated, Goal-Oriented Materials Discovery



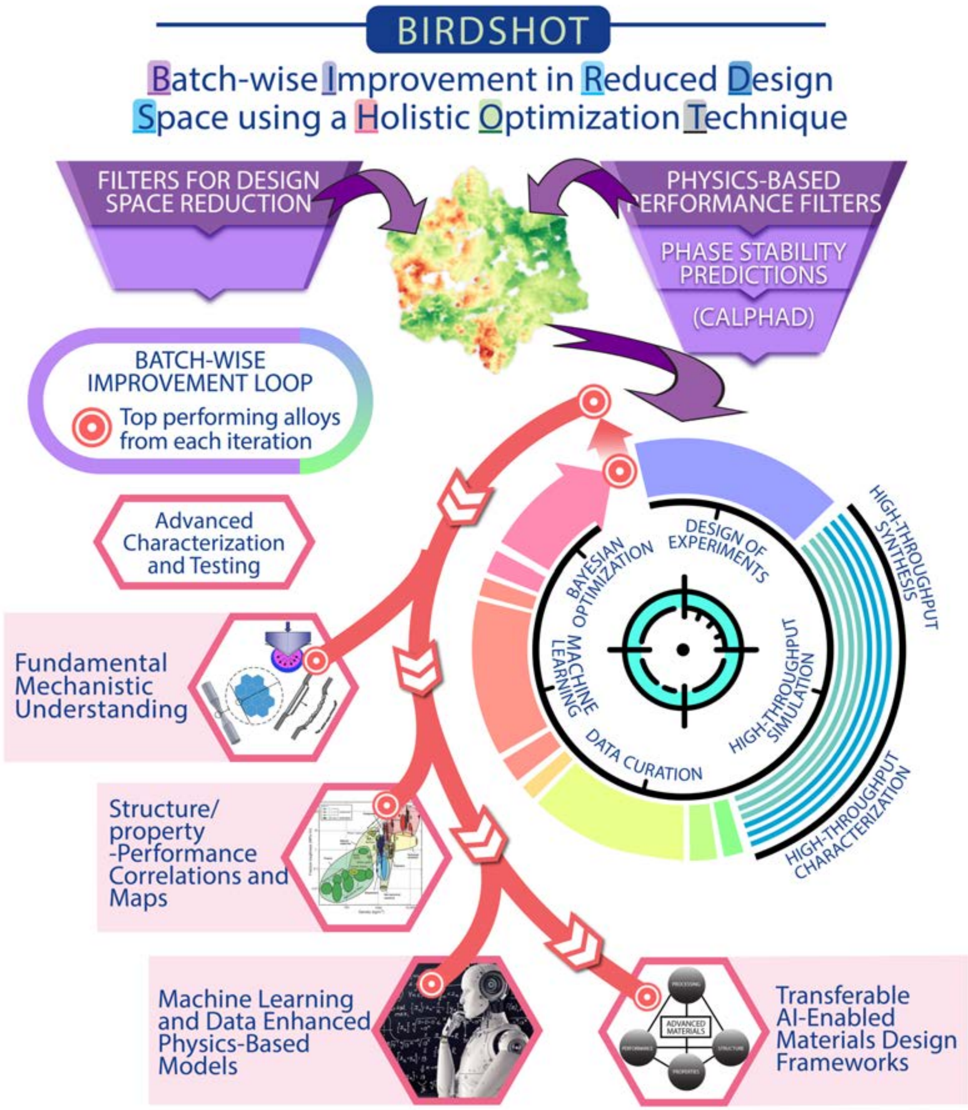


For Agile War Fighter Technology Development

BIRDSHOT CAPABILITIES PORTFOLIO

- ARMY+ARL Partners
  - Identify Army Requirements & Responsive R&D
  - Inform and Collaborate in Research and Transitioning
- TAMU+GTECH+UCSD:
  - Beyond SOA High-Throughput Synthesis of Advanced Army-relevant Materials
  - World-unique HTP Characterization of Materials' Response under *EXTREME CONDITIONS*
  - Best-in Class AI/ML Enabled Materials Discovery/Design Frameworks
  - Highly Integrated Multi-Scale Modeling Capabilities
  - Efficient Integrated Center-wide Data Management Tools
- **INDUSTRY PARTNERS**:
  - Provide Needed Core Competencies in Scale-up and Commercialization
  - Collaborate in Research
  - Co-invest in the Center

The BIRDSHOT Way

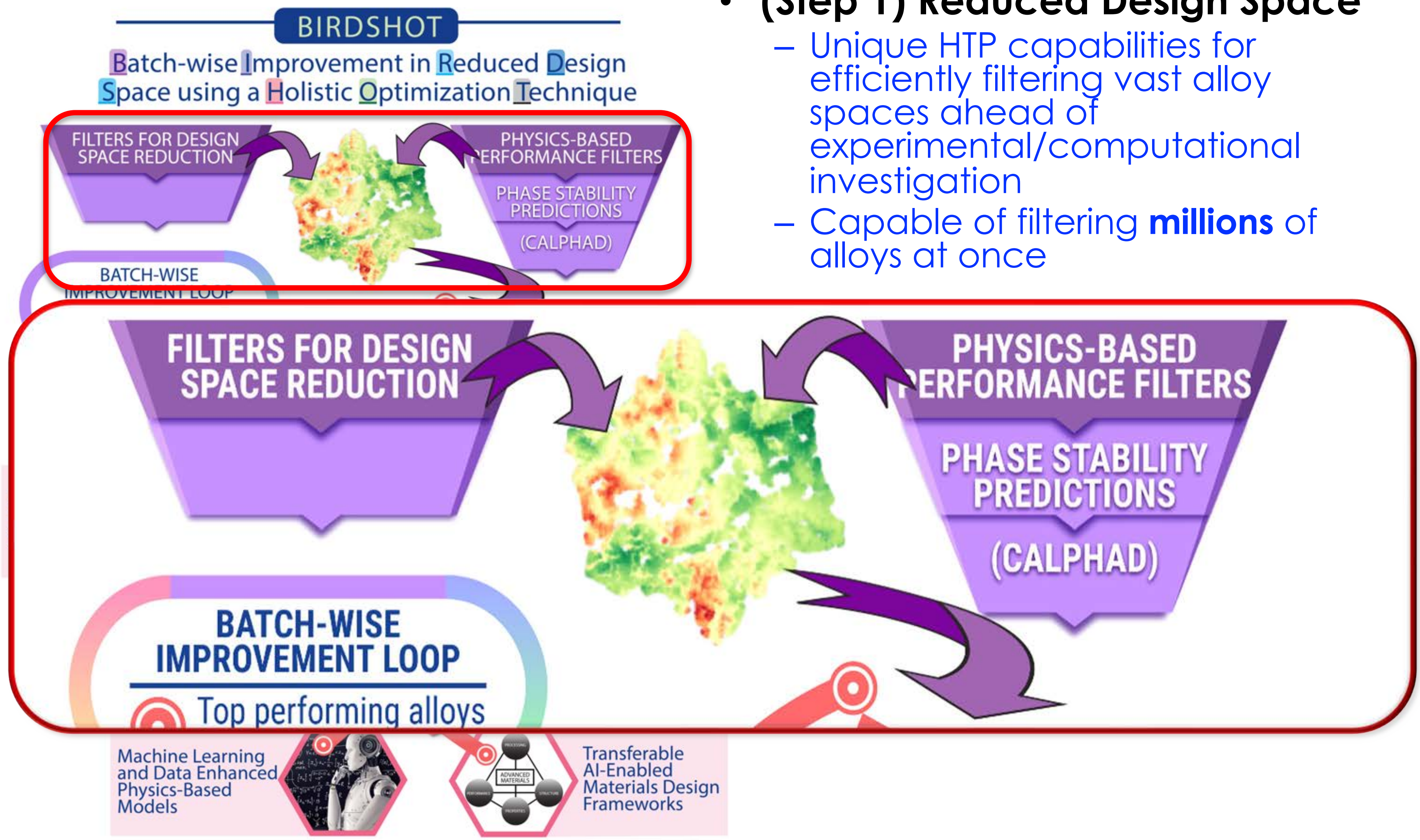


BIRDSHOT Approach:

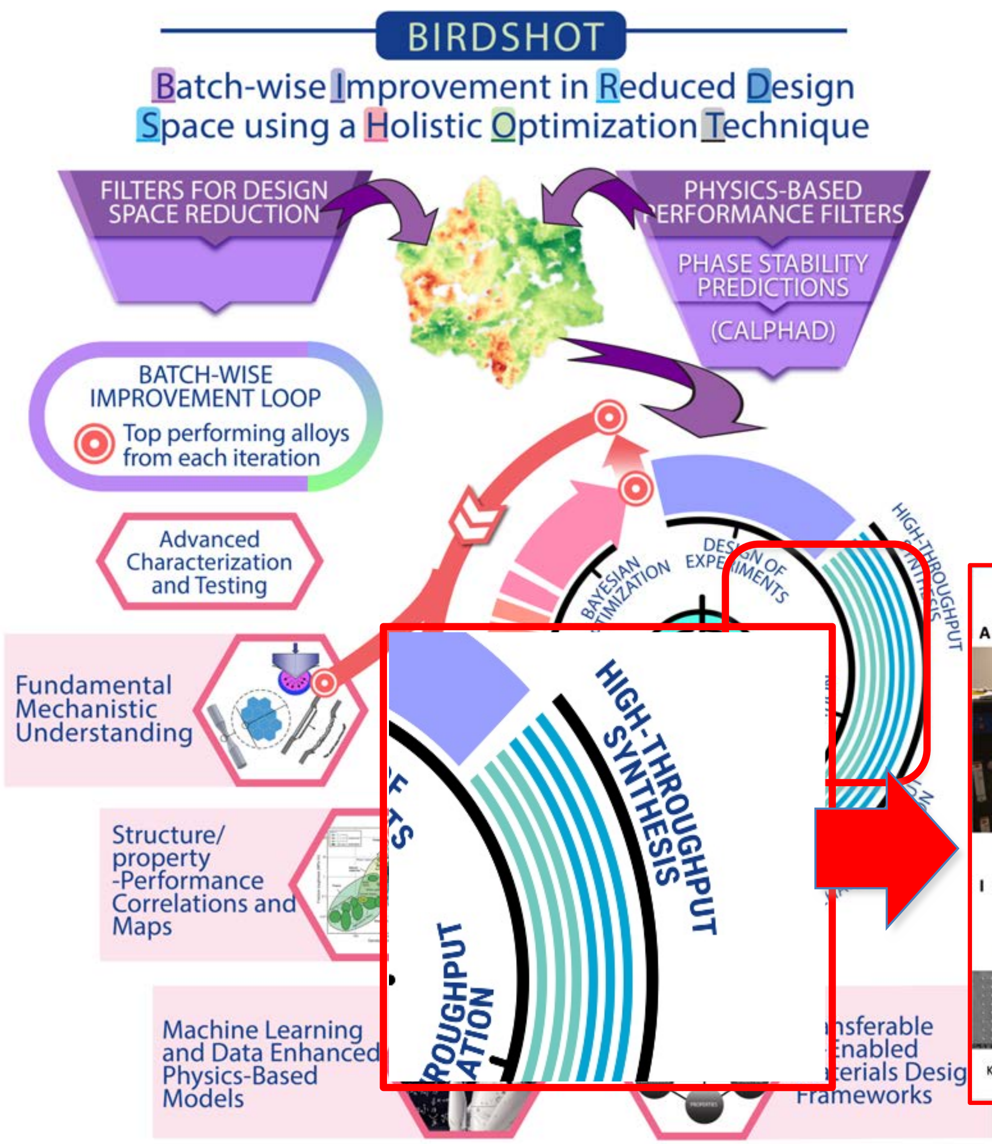
- **Step1**: Filter Alloy/Materials Space
- **Step 2**: HTP Synthesis
- **Step 3**: HTP Characterization (Extreme Conditions)
- **Step 4:** HTP Simulations
- **Step 5**: Optimal Learning of Physics of HSR Deformation
- **Step 6**: Deploy Multi-Information Source Batch Bayesian Optimization

HTP Screening (Arroyave)

- **(Step 1) Reduced Design Space**
  - Unique HTP capabilities for efficiently filtering vast alloy spaces ahead of experimental/computational investigation
  - Capable of filtering **millions** of alloys at once

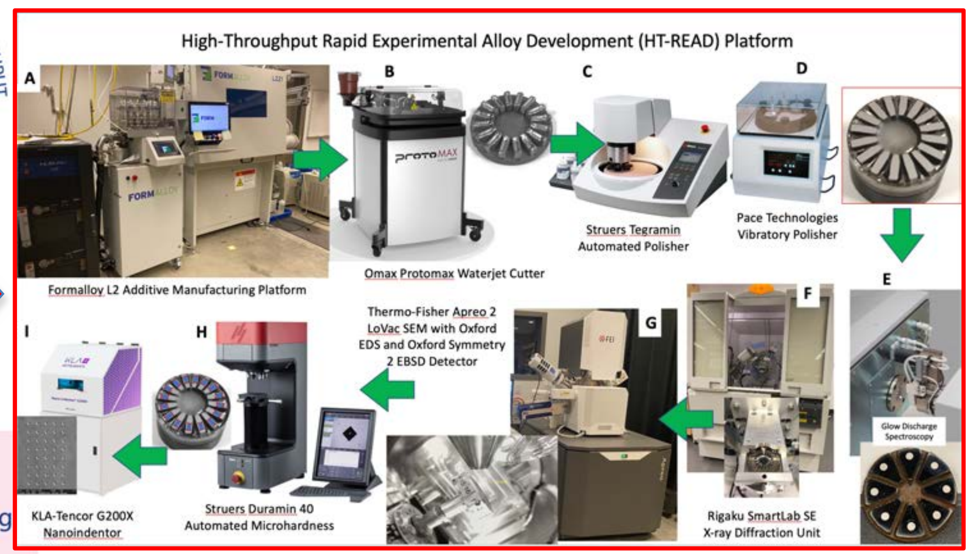


HTP Synthesis (Vecchio, Karaman)

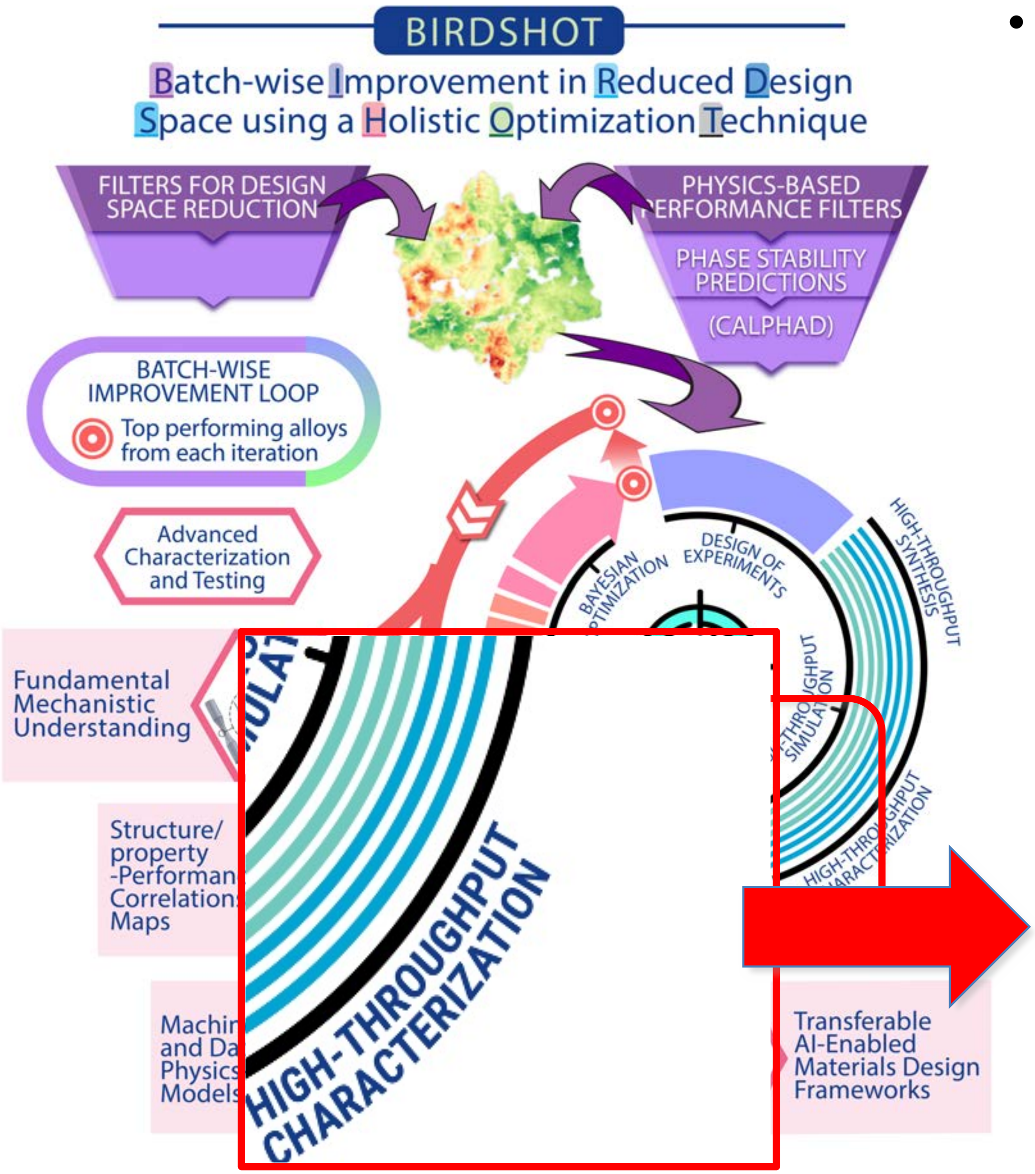


- **(Step 2) HTP Synthesis**
  - Highly integrated, beyond SOA HTP synthesis and preparation platform
  - (DED-based Alloy Prototyping)

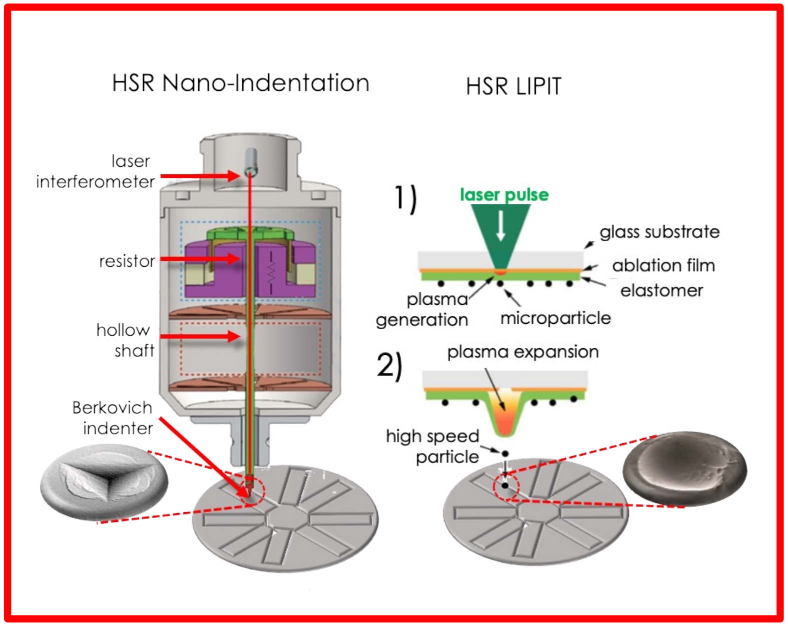
HT-READ



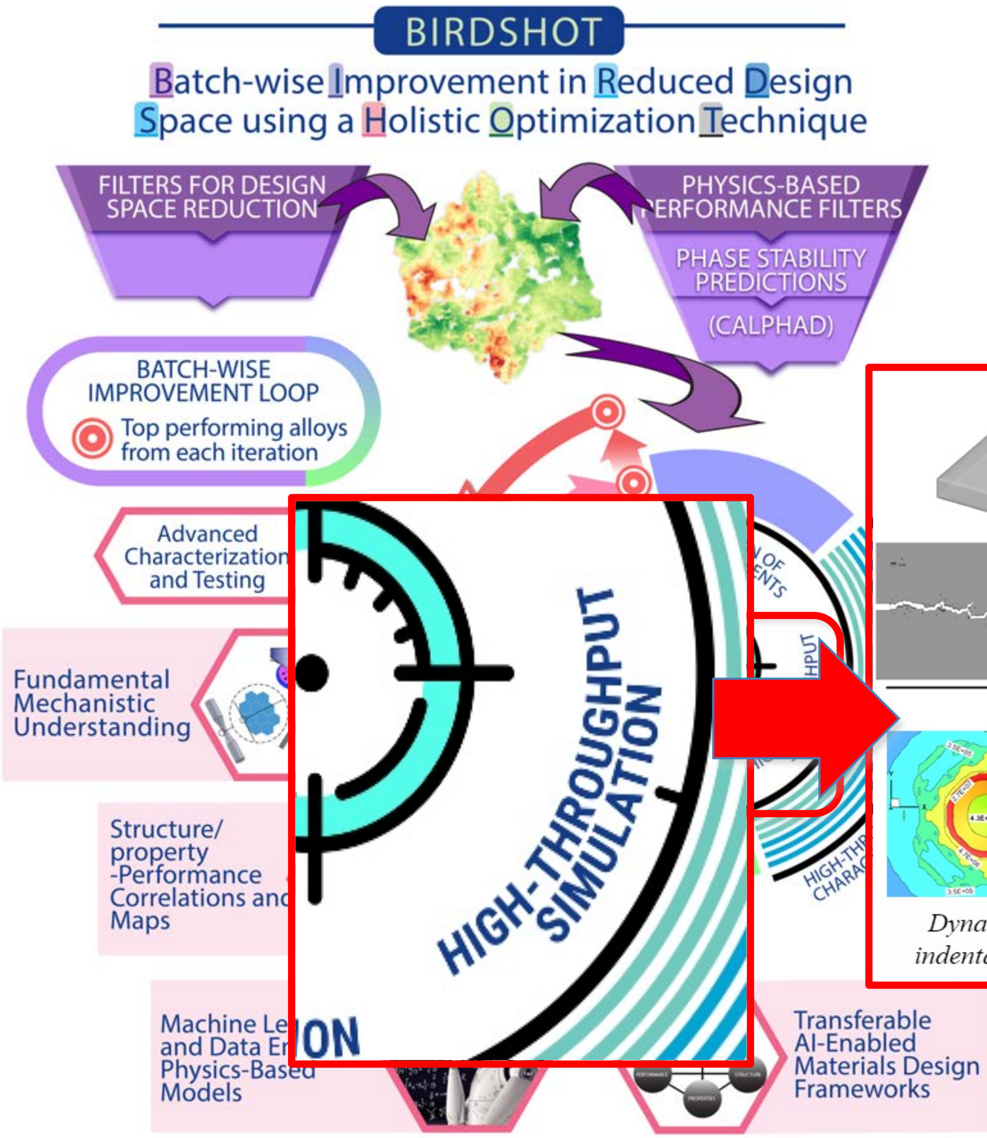
HTP Characterization (Pharr, Thomas)



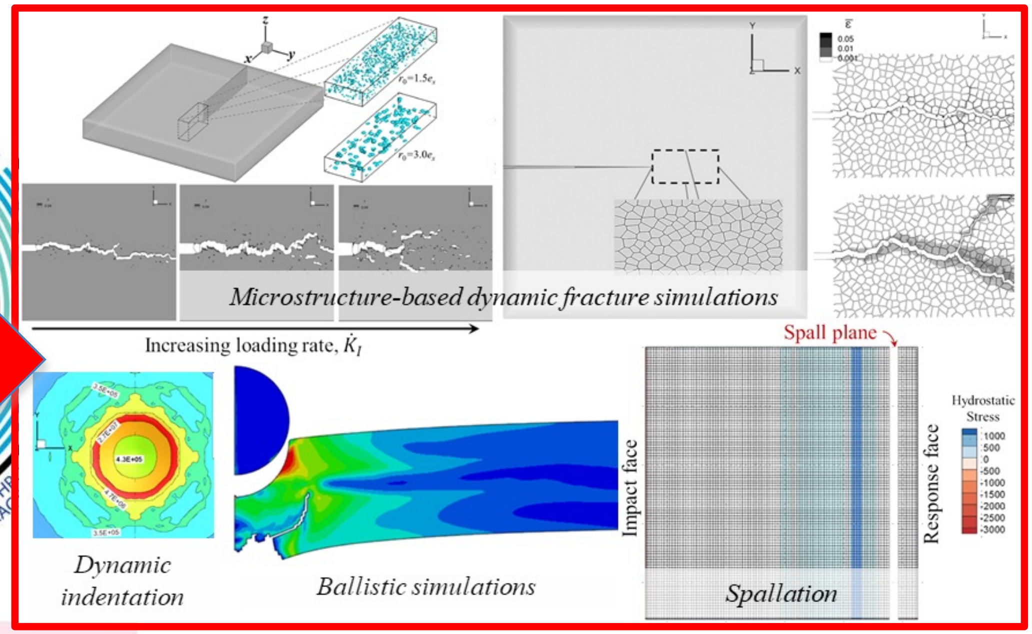
- **(Step 3) HTP Characterization**
  - HTP nano indentation at high-strain rates and temperatures (Pharr)
  - HTP Laser Induced Particle Impact Testing (LIPIT) (Thomas)
  - Strain Rates: 10^3-10^8/s
  - Other extreme conditions (i.e. high temperature, oxidation, etc.)



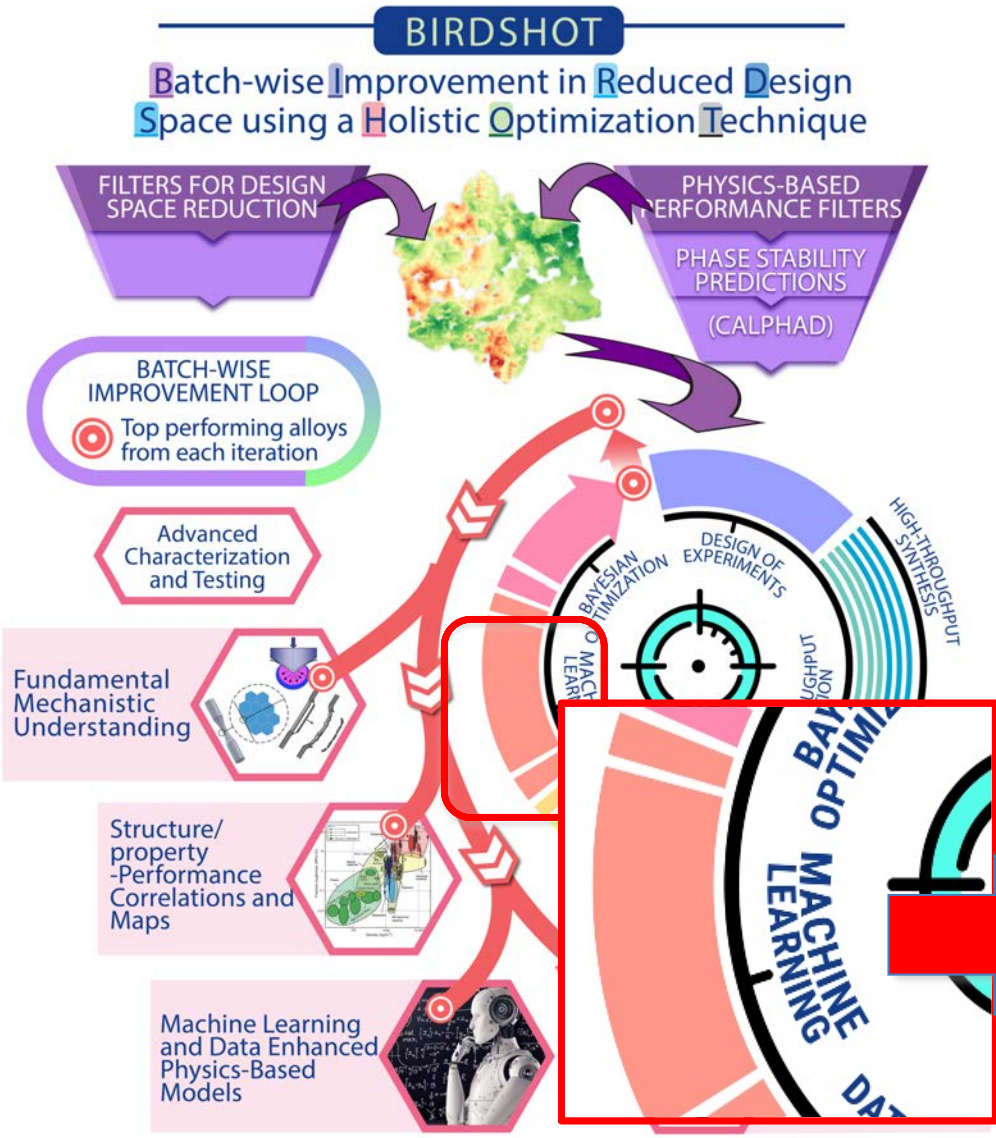
HTP Simulations (Srivastava)



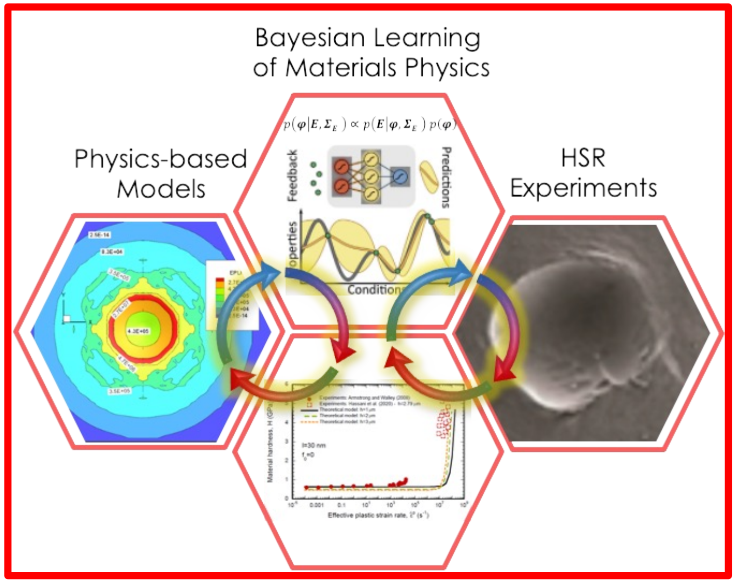
- **(Step 4) HTP Simulations**
  - Advanced simulations of HSR deformation of materials
  - ML-enabled Scale Bridging



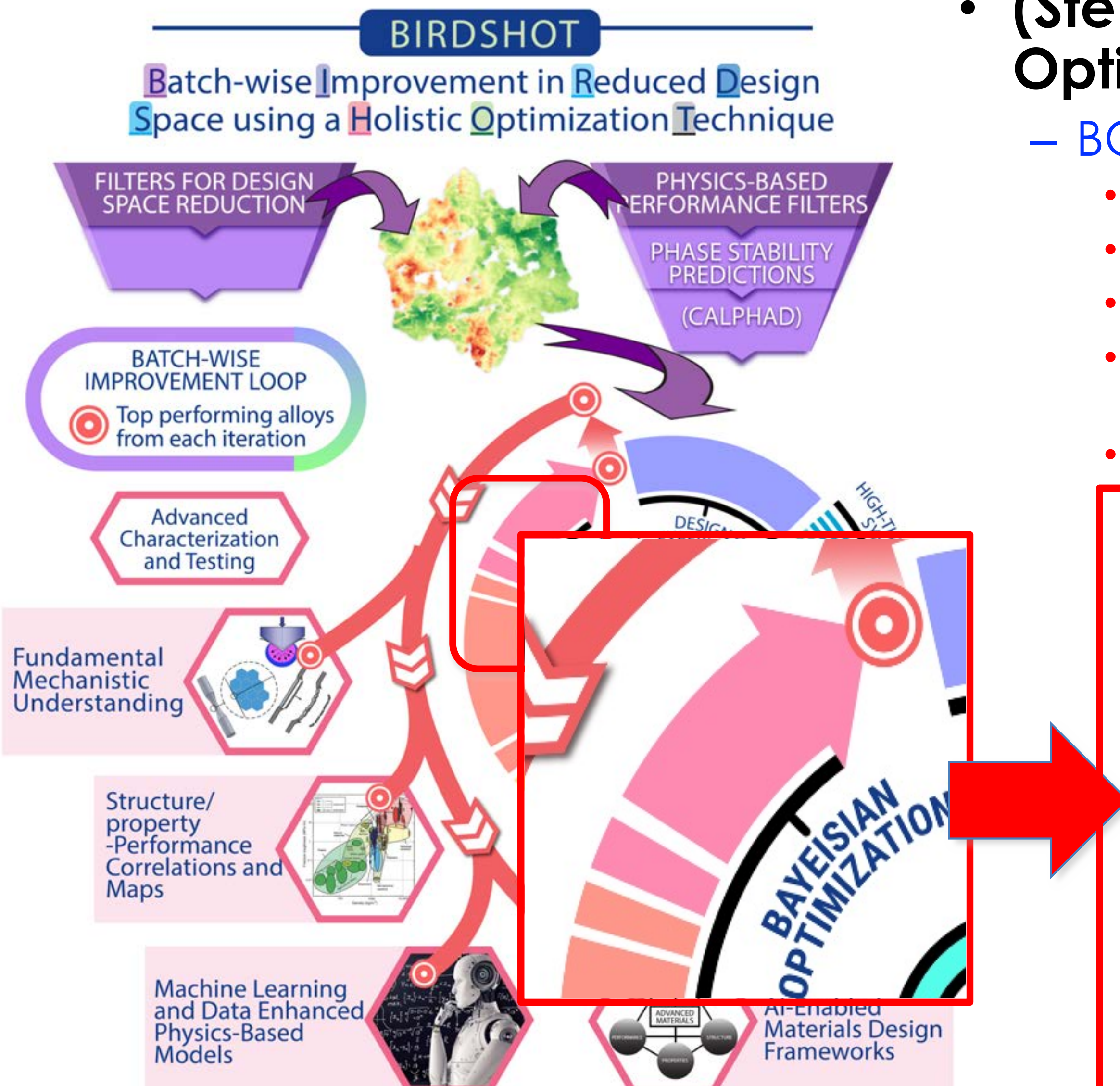
Optimal Learning (Srivastava, Kalidindi, Arroyave, Allaire)



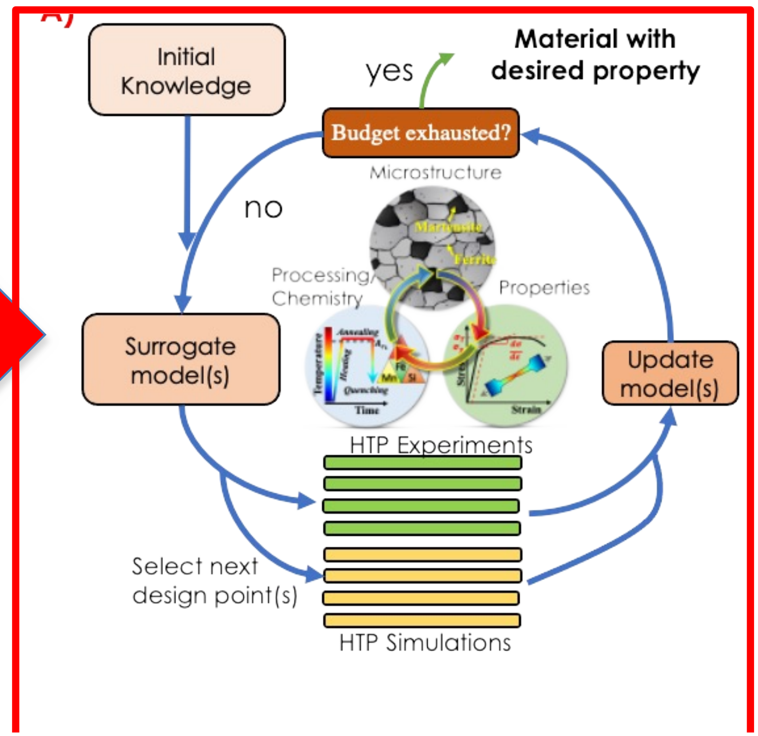
- **(Step 5) ML-Physics Coupled Models**
  - Bayesian approaches for accelerated learning of physics of HSR deformation
  - Enabled by Physics-Constrained Fast-Acting ML Surrogate Models



Bayesian Optimization (Srivastava, Allaire, Arroyave)



- **(Step 6) Bayesian Optimization**
  - BO Capabilities:
    - Sparse data sets
    - Multi-Information Source
    - Multi-Objective, Multi-Constraints
    - Batch (to account for parallel experiments)
    - Microstructure Aware



Workforce Development

Computational Materials Science Summer School:

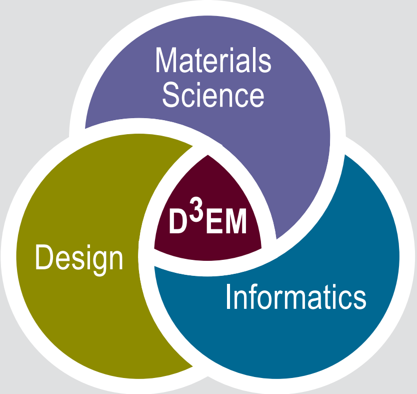
CMS³

D³EM Program:

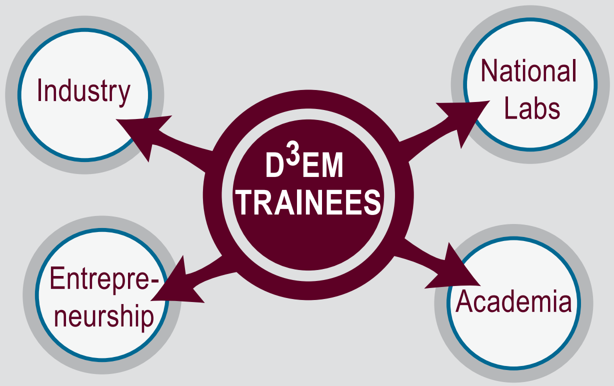
SIX DEPARTMENTS • THREE DISCIPLINES • ONE VISION

Building a collaborative framework for the accelerated development of materials through materials science, informatics, and engineering design.

TRANSCEND DISCIPLINES



LAUNCH SUCCESSFUL CAREERS



IMPACT ENERGY TECHNOLOGY & SYSTEMS

MATERIALS FOR:

- Energy Storage
- Energy Conversion
- Sustainability
- Energy Efficiency

Our Vision: An Autonomous Materials Research & Development Platform

TEXAS A&M UNIVERSITY
Engineering

Texas A&M Engineering
Experiment Station

TEXAS A&M UNIVERSITY

GEORGIA TECH

UC San Diego

THANKS!