Stage 1 Readiness

Due Monday February 9th

Project 1 — Optimizing High-Entropy Diboride Coatings (AFLOW)

High Entropy Diboreds
Diboride Coatings
Data from AFLOW, use BLADE or materialsframework
Properties: Thermal expansion, melting point, high hardness, oxidation resistance, thermal stability, bond compatibility.
SNPS: We need more efficient engines. One way to increase efficiency of engines is to increase inlet temperature of the engine. Current material systems for blades peaked around 1500C. There is a need for new coatings.

Project type **(choose)**:

- **Optimization/Design**: Find a material or process that maximizes/minimizes a property
- Predictive Tool: Build an accurate model to predict a property from features
- Screening/Classification: Identify or classify candidate materials
- Understanding/Discovery: Identify key features or relationships governing behavior

Design Variables & Goals

- Data acquisition: AFLOW
- Design variables: Compositions
- Objectives: E (max), Thermal Stability (max), Specific Stiffness (max), Formation Energy (min), Cost (min)
- Constraints on inputs: List of components
- Constraints on objectives: Toughness > X

Project 2 — Fusion Reactor 2nd Blanket Material (thermal/structural + activation metrics)

Find a material to make a 2nd blanket for a fusion reactor. Needs to withstand temperature, cannot let heat pass through to the 3rd layer. Does not need to directly withstand irradiation exposure.
Structural, heat, mechanical load.
DPA damage per atom. This is a metric of radiation damage and exposure.
Neutron flux. Look up common neutron fluxes for DEMO and ITER and neutron spectra.
H2 generated after exposure to a certain spectra
He generated after exposure to a certain spectra
H3 generated after exposure…
Activation properties, bq, dose, waste and disposal
Yield strength at high temperature 500C to 700 C
Creep with cyclical temperature loading
Frankle pair recombination rate
SNPS: ?

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Design Variables & Goals

- Data Acquisition: Find 3D models and use OpenMC
- Design variables: Creep resistance, ductility, production of gas byproducts, more
- Objectives: structural (yield strength), efficiency (heat transfer and neutron transfer)
- Constraints on inputs: Material Selection

Project 3 — MOSN Materials

New project

Project type **(choose)**:

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Design Variables & Goals

- Data acquisition: DFT Simulations
- Design variables: Composition of functional groups (2) and Position
- Objectives: Band Gap close 1.3 (“Error”=|Band Gap - 1.3|, min), Elastic Modulus (max)
- Constraints:

Project 4 — Predict Solidification Microstructure (dendritic vs planar; any geometry)

Making a framework that can predict the microstructure, dendritic formation / planar formation based on how an alloy solidifies. It could work for any geometry.
SNPS: Process-structure-property-performance is the cornerstone of materials design but making linkages across this chain are done at great cost. Design of microstructure is important but is often treated as an intermediate variable. Cast materials are widely used but suffer from mechanical performance based on how they cool down. A factor in that is the solidification path. We need a tool to predict how microstructure could solidify and from that we can predict some properties.
SNPS: Cast microstructure is bad because there is a gradient, there is difference in microstructure across the length scale, and there is segregation because of dendrites and different solidification morphology.
Casting steel, there is a high chance of forming pores.
SNPS: [Find a case or problem that was caused by poor properties in cast material but frame it as a performance issue first.]
Casted materials occasionally suffer from poor performance.
HEAs, you can tune the properties using SRO. SRO can be tuned by processing parameters.

Active learning

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Design Variables & Goals

- Data: Thermocalc
- Design variables: (Composition), Env Temp During solidification, Sample Geometry
- Objectives: 3D map of the sample (dendritic/planar)
- Constraints: Arc melter configuration, maybe composition

Project 5 — Eyewear Polymers: High Refractive Index for Thinner Lenses (project type question included)

Optimize better eyewear using new classes of polymers, high refractive indices (customize, control), minimize thickness (style). User input idea. I wanted glasses with bad eye sight, and I want thinner lenses.
Populations of people with certain eye issues.
Variables:
UV, Strength, Thermal conductivity, Refractive index, Cost, Coatings to reflect certain wavelengths.

Project type **(choose)**:

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- Screening/Classification: Identify or classify candidate materials
- Understanding/Discovery: Identify key features or relationships governing behavior

Design Variables & Goals

- Data acquisition: Databases of refractory indexes and polymer cost
- Design variables: budget, material selection, geometry
- Objectives: Thickness (min), mechanical durability (max)
- Constraints: Manufacturability, **Does the lens work (refractory index)**

Project 6 — LLMs to Accelerate Bayesian Optimization (text + expert intuition)

In BO, in any materials engineering problem, can we use LLMs to accelerate BO? In a lot of scenarios a lot of info is in text and not available in mathematical terms, can we use LLMs to encode this info in BO. Can we incorporate preferences and rules of thumb and intuition from (Dr. Karaman) a human in the loop. Intuition. LLM can search through literature and get intuition from experts.
SNPS: It takes an expert 10,000 hours

Project type **(choose)**:

- Optimization/Design: Find a material or process that maximizes/minimizes a property
- Predictive Tool: Build an accurate model to predict a property from features
- Screening/Classification: Identify or classify candidate materials
- **Understanding/Discovery**: Identify key features or relationships governing behavior

Design Variables & Goals

- Design variables: Papers, books, charts
- Objectives: Prior function on some property
- Constraints: Will design use cases and they will have different constraints

Project 7 — Carbon Fiber Structural Batteries

New project

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- Predictive Tool: Build an accurate model to predict a property from features
- Screening/Classification: Identify or classify candidate materials
- Understanding/Discovery: Identify key features or relationships governing behavior

Design Variables & Goals

- Data acquisition: COMSOL, Python Libraries
- Design variables: 12 variables
- Objectives: Energy Capacity (max), Stiffness (max), Strain (min), Life Cycle (max)
- Constraints **Fill**