Project 1:
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 2:
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: ?

Project 3:
Electron-phonon coupling, Hamiltonian for superconductivity in material.
First use DFT to provide training data. Use a training dataset to fine tune a ML model, and use this model to predict material with properties for superconductivity.
Structure, calc Hamiltonian, so phonon maps input structure to Hamiltonian, and then decides if it can be used for superconductivity.
Find relationships with input structure and Hamiltonian. If we know the Hamiltonian, we can determine if something is superconducting or not.
How do I actively learn the relationship between input structure and Hamiltonian? Bayesian active learning.
SNPS: Energy efficiency crisis, environmental. A potential solution could be finding superconducting material. However, the current issue in science is that we don't have a fast way to screen for candidate materials structures to find their Hamiltonian which tells us about their superconductivity.
Active learn the structure-property-performance chain.

Project 4:
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.
(Sushant) 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.
(other) 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.

Project 5:
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 6:
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 7:
Best alternative material to replace Li, focus on properties, application, and performance. We want to consider fast charging.
17 materials (organic and inorganic)
Has a list of properties. (At least 8)
SNPS: Charge fast and discharge in a longer period of time.