Metallic glasses are an emerging class of materials with highly unique and desirable properties. A difficulty in the production of metallic glasses is the necessary cooling times. Metallic glass is an amorphous phase of matter composed of elements that would normally form ordered metallic crystals. The crystal phases are extremely favorable at low temperatures, so the atoms must be trapped in the amorphous phase before they can rearrange. This requires a rapid transition from the liquid phase (often a very high temperature for metals) to temperatures below the glass transition, too low for atoms to be mobile. I propose using Mechanistic Data Science principles and methods to create a model that predicts the glass transition temperatures of alloys.

1. Data collection and generation
   1. <https://www.kaggle.com/saurabhshahane/metallic-glass-forming>
      1. This dataset contains relevant data for glassification.
   2. <https://www.kaggle.com/jwaitze/tablesoftheelements>
      1. This dataset contains additional data for every element
   3. <https://materialsproject.org/>
      1. Materials project contains compound data for crystal structures
   4. As an undergraduate student in the MatSci department, I have access to advanced thermodynamics software and databases.
2. Mechanistic feature extraction
   1. Things such as Tg, melting points, elemental composition, properties of the elements, electron configurations, atomic radii, equilibrium packing structure, nearby phases, and many more properties
3. Dimension reduction
   1. I will consult my MatSci course notes for as many relations as possible that I can use to reduce the number of independent features
   2. If necessary, I will use surface-level regression to see if there are any evident feature correlations that were not included in my background knowledge.
4. Mechanistic learning through regression
   1. I will have to see what computational resources I would have access to, but neural networks seem like a very obvious choice for this given the highly complex interactions between atoms.
5. Reduced-order surrogate models
   1. Molecular dynamics simulations are the ideal computational method for modeling glass transitions. Again, highly dependent on available computational resources.
6. System and design
   1. Use the model to predict the glass transition temperatures of alloys with little/no existing glass transition data.