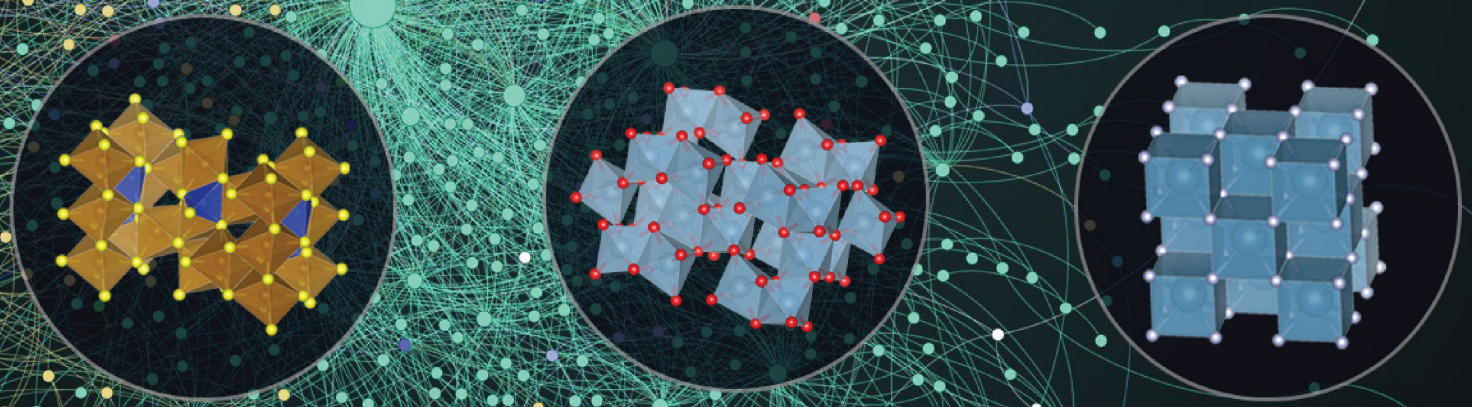
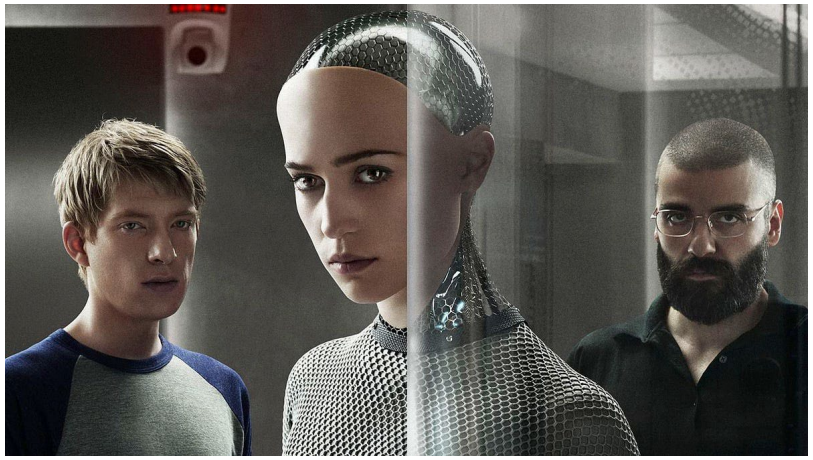
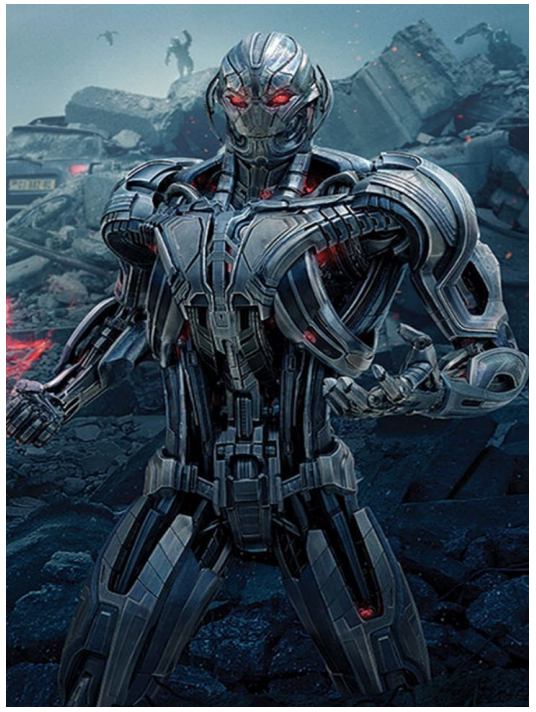
# Featurization in Materials Informatics



# AI in movies is often portrayed as cold and logical







# How will ML know what to do if we provide no instruction?

“The dog has been in the habit of carrying this stick behind his master. Being a heavy stick the dog has held it tightly by the middle, and the marks of his teeth are very plainly visible. The dog's jaw, as shown in the space between these marks, is too broad in my opinion for a terrier and not broad enough for a mastiff. It may have been – yes, by Jove it is a curly-haired spaniel.”

# Features should be correlated with the target label

In machine learning and pattern recognition, a feature is an individual measurable property or characteristic of a phenomenon.

Choosing informative, discriminating and independent features is a crucial element of effective algorithms in pattern recognition, classification and regression.

# Features should  be correlated with the target label


Shoe size (inches)
Shoe size (cm)
Age
Favorite food
Race
Shirt Color
Gender
Zip Code
Asleep/Awake
Genome sequence
Occupation
Eye color
Weight

# Not all features are equally important


Shoe size (inches)
Age
Gender
Weight
Race
Genome sequence (highly complex)
Occupation (weak?)
Eye color (weak?)
Zip Code (weak?)
Shoe size (cm) (not independent)
Favorite food (no correlation)
Shirt Color (no correlation)
Asleep/Awake (no correlation)

# Some ML algorithms can even tell us features weight!

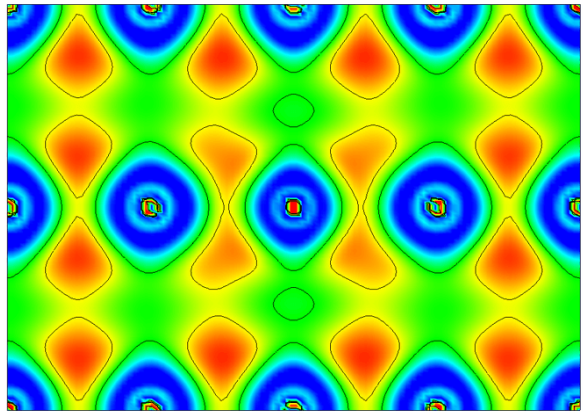
# Featurization is not the same as feature engineering

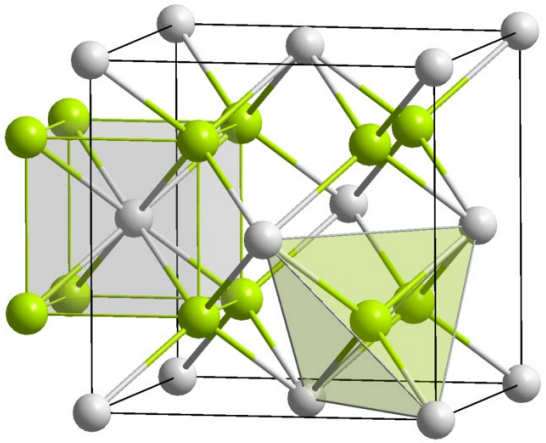
Featurization is a way to change some form of data (text data, graph data, time-series data,…) into a numerical vector.

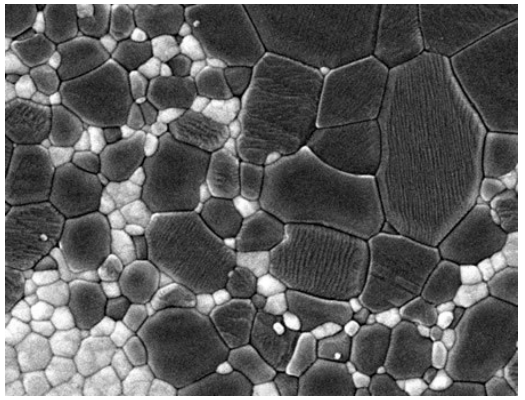
Featurization is different from feature engineering. Feature engineering is just transforming the numerical features somehow so that the machine learning models work well. In feature engineering, features are already in the numerical form, whereas in featurization data not need to be in the form of numerical vector.

# What soft of materials features do we have to pick from?

Electronic → Atomic → Microstructure → Macroscale







# Composition-based feature vector