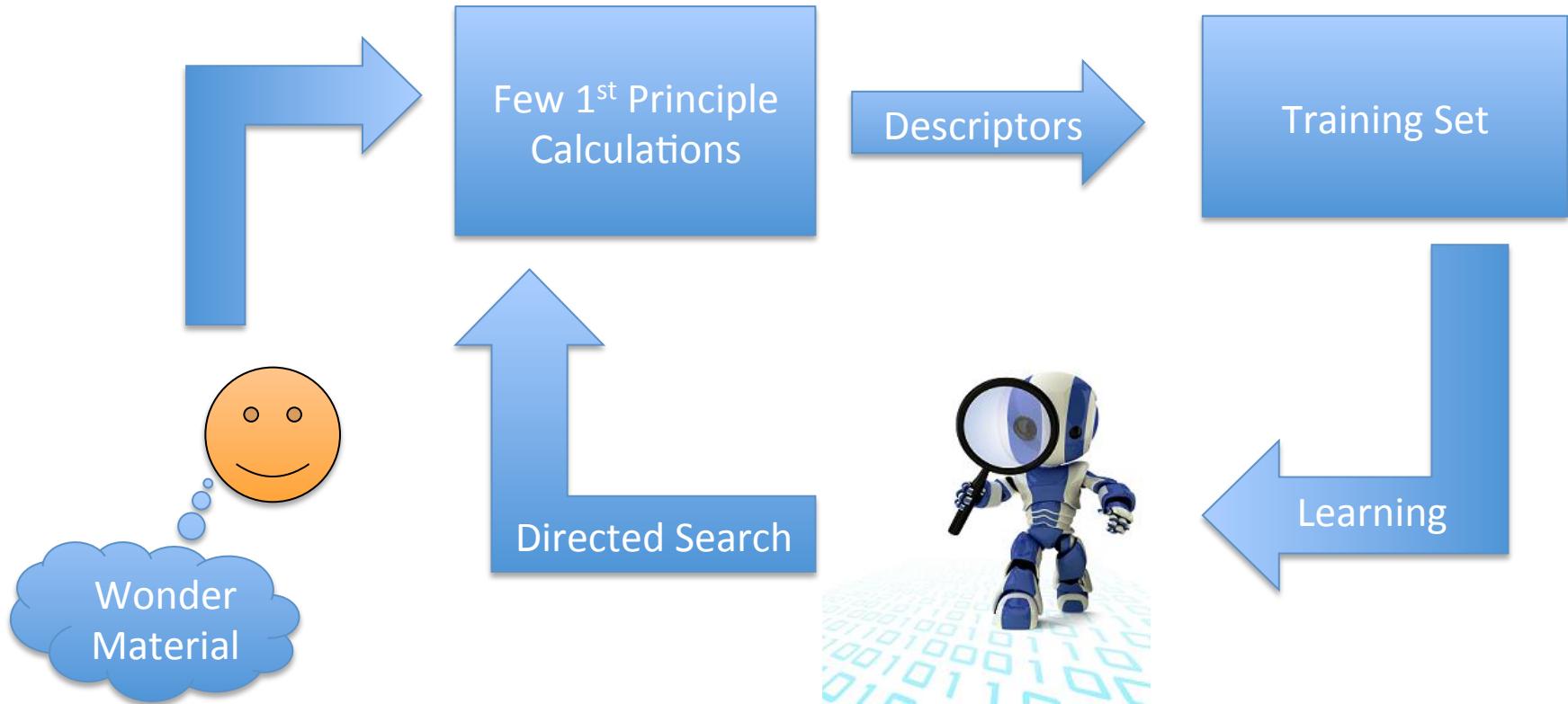


# Materials Properties from Machine Learning

Andrew Long  
Ioan-Bogdan Magdau

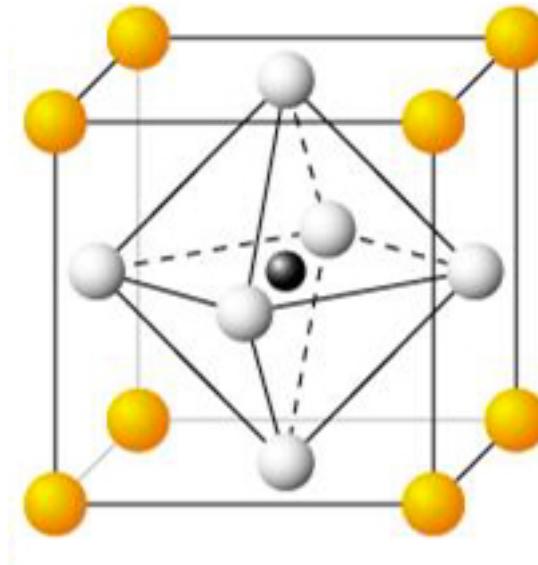
# The Idea



# Proof of Concept

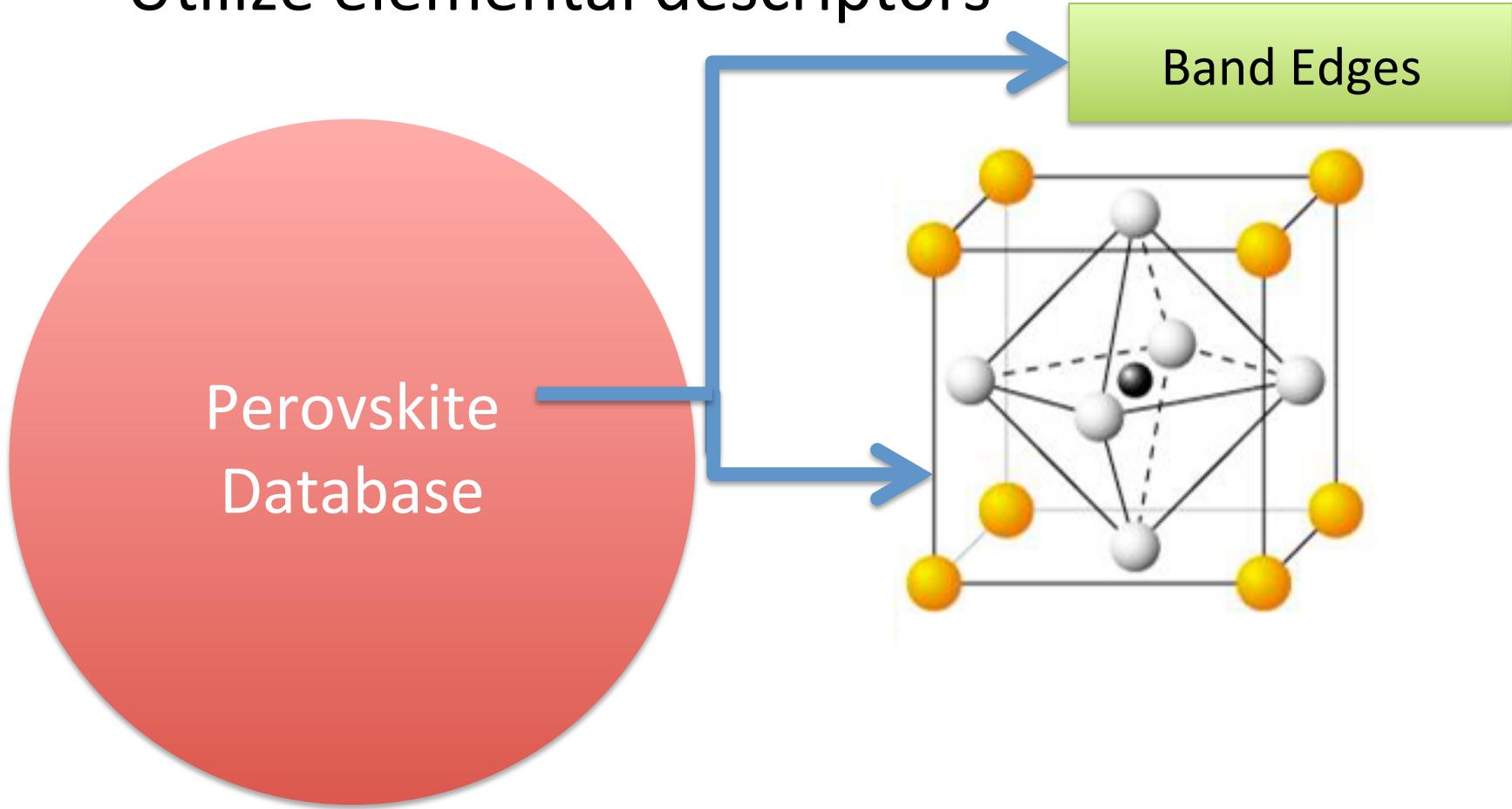
- Simple linear regression to predict electronic band extrema?

Perovskite  
Database



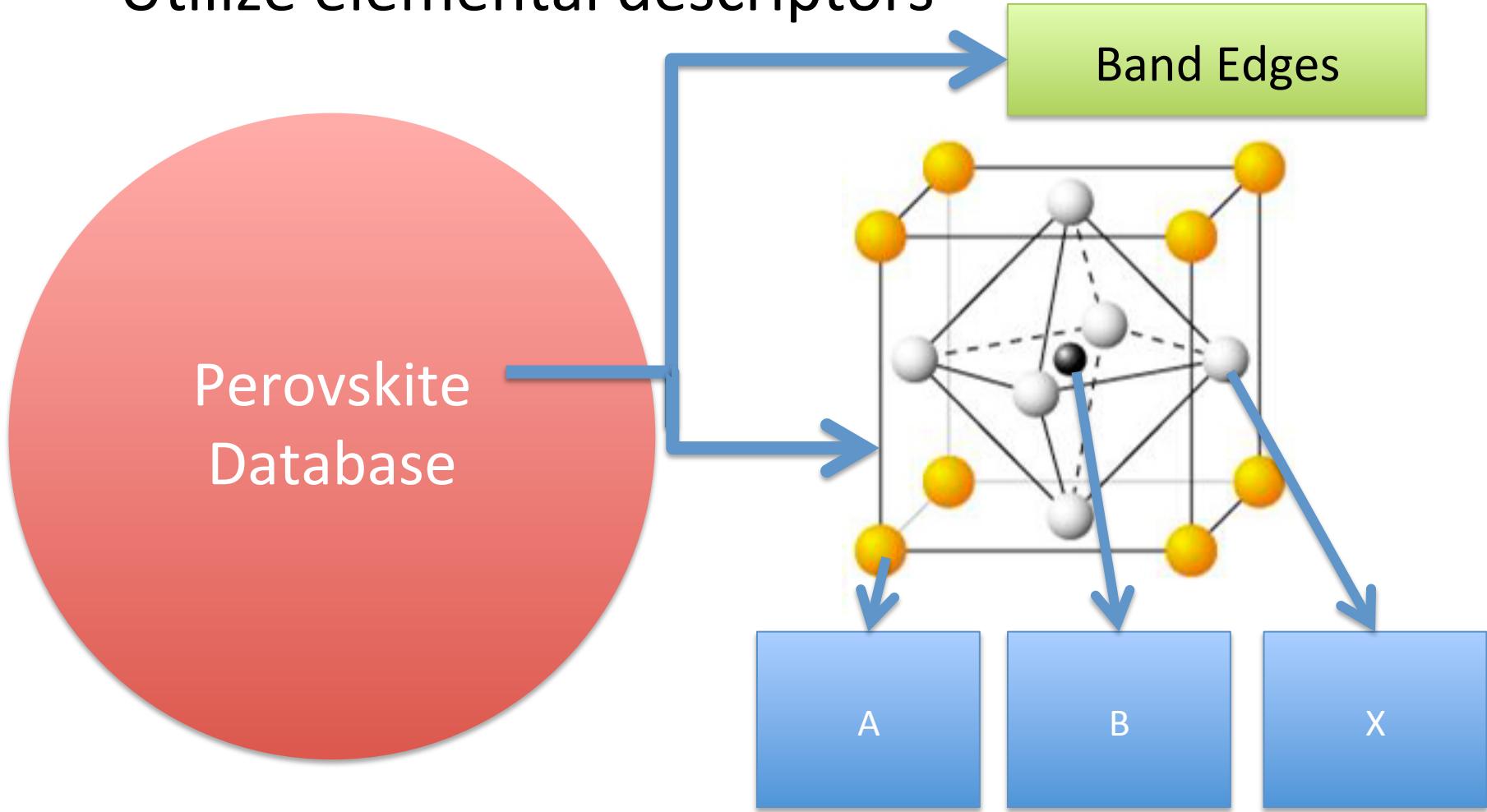
# Proof of Concept

- Utilize elemental descriptors



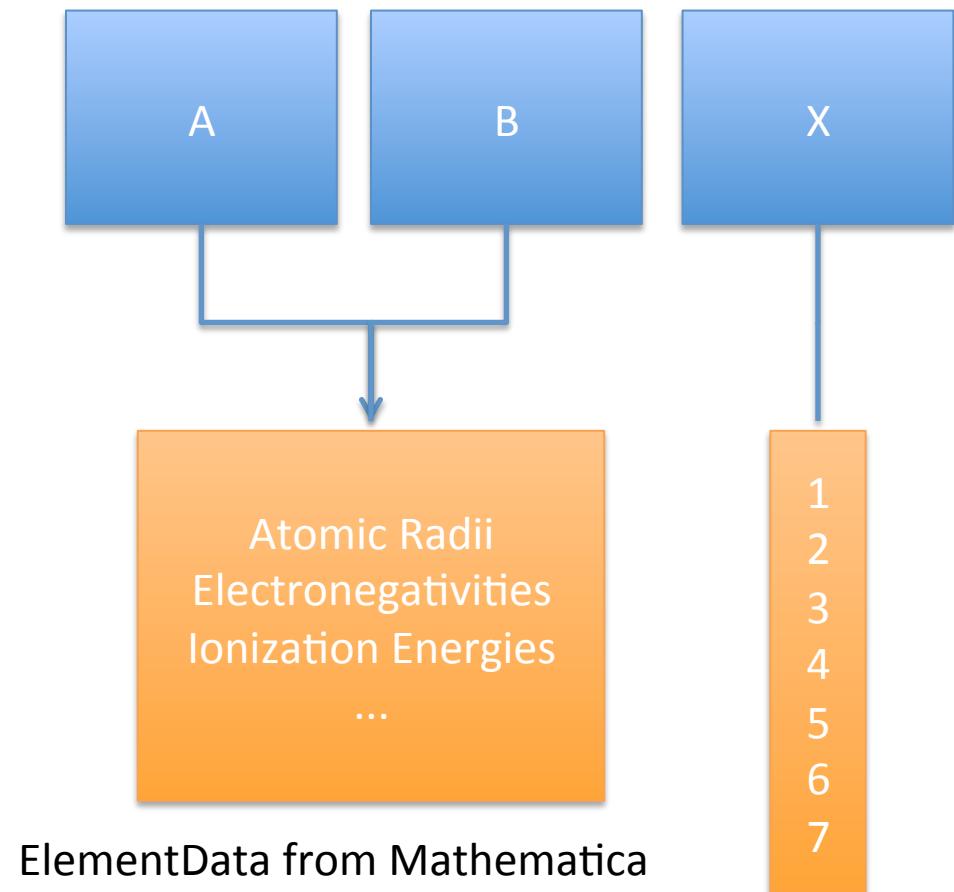
# Proof of Concept

- Utilize elemental descriptors



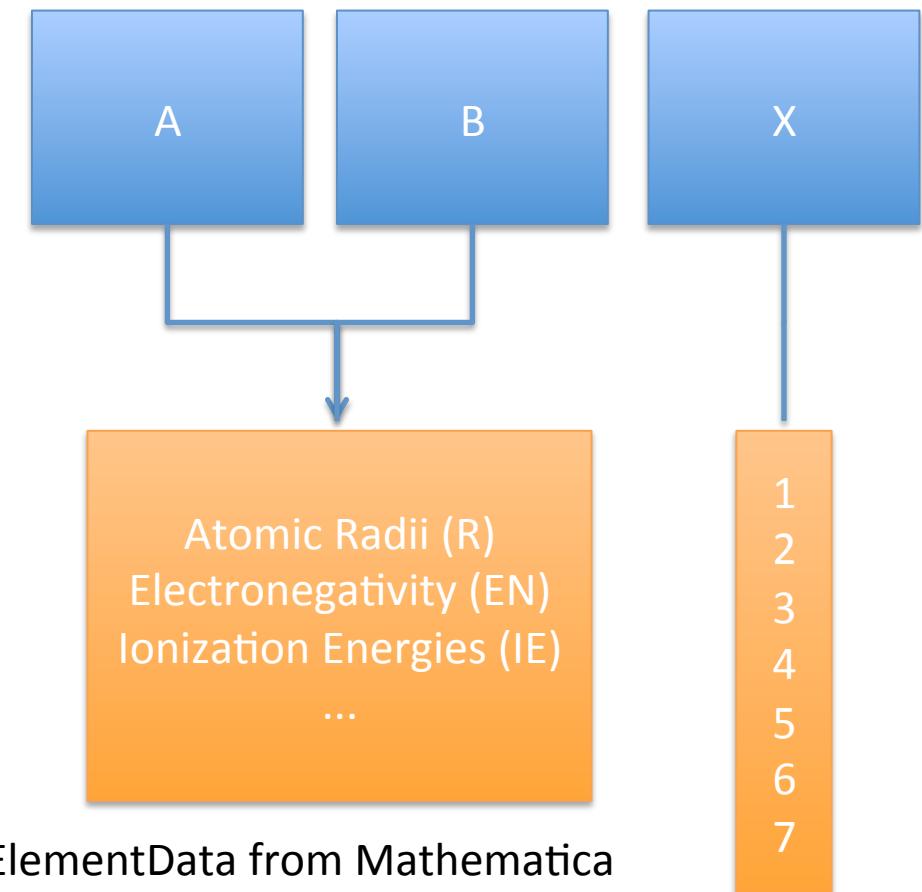
# Proof of Concept

- Utilize elemental descriptors



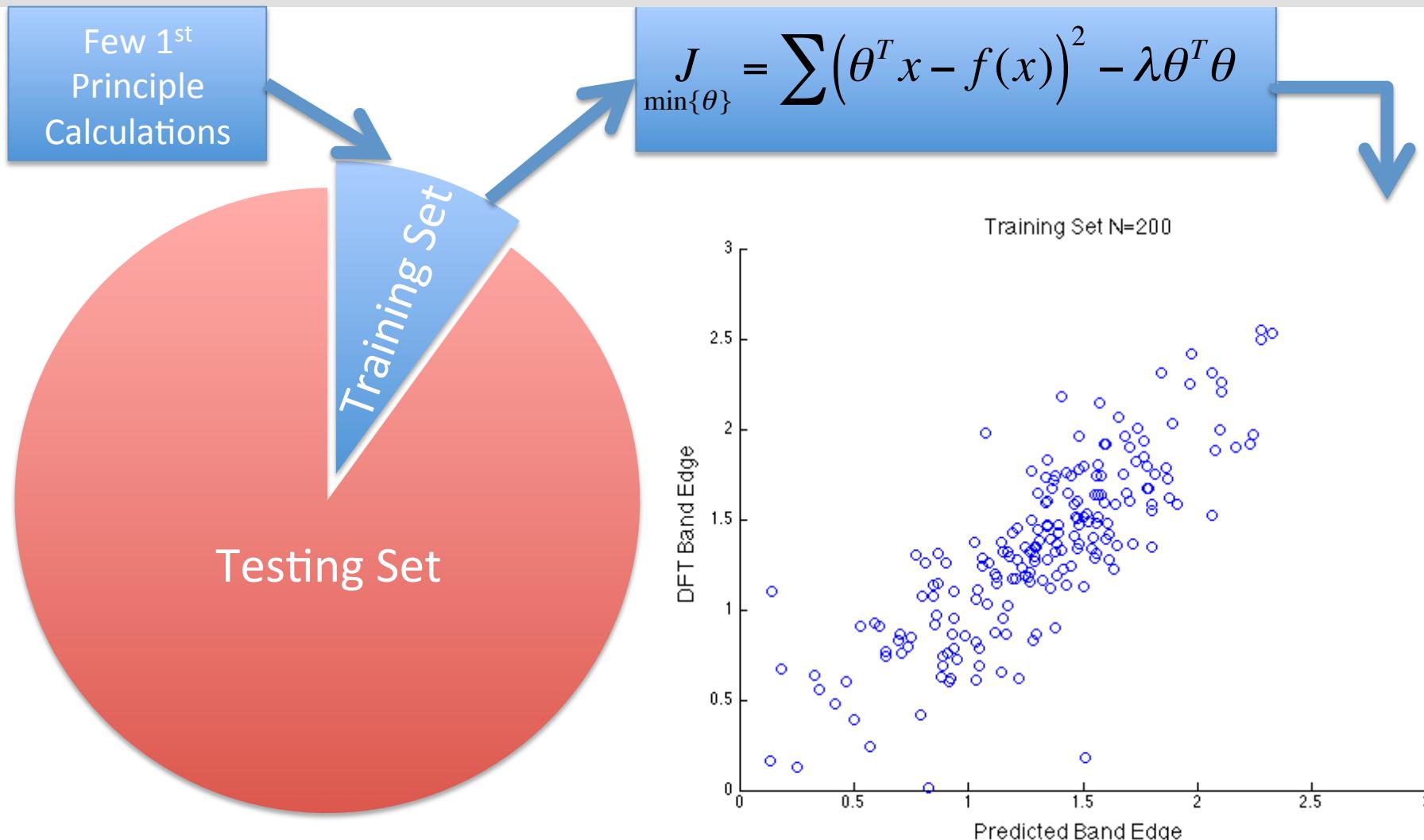
# Proof of Concept

- Utilize elemental descriptors



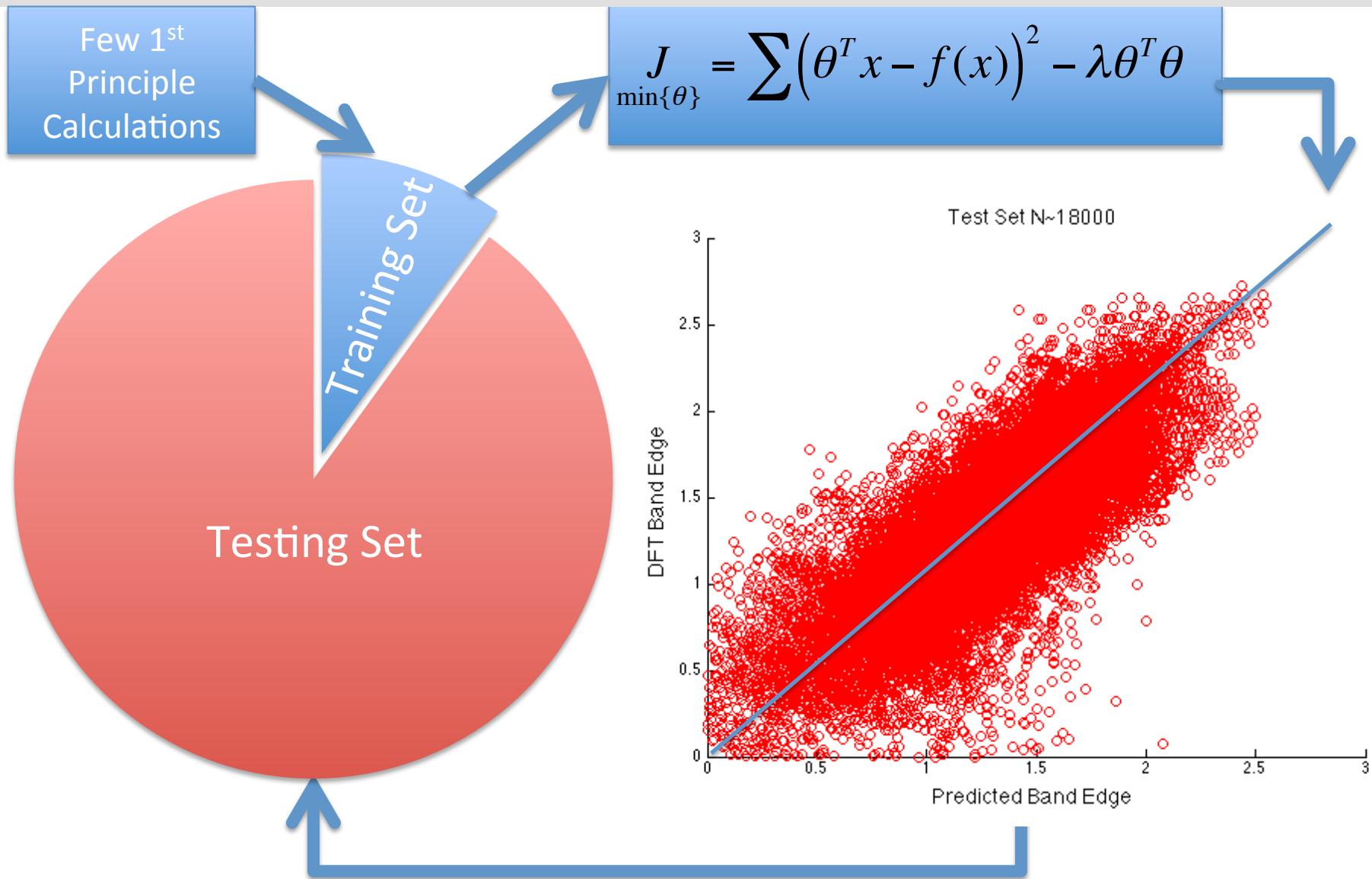
$$BandEdge = f(A(R, EN, IE, \dots), B(R, EN, IE, \dots), X)$$

# Proof of Concept



$$\text{BandEdge} = f(A(R, EN, IE, \dots), B(R, EN, IE, \dots), X)$$

# Proof of Concept

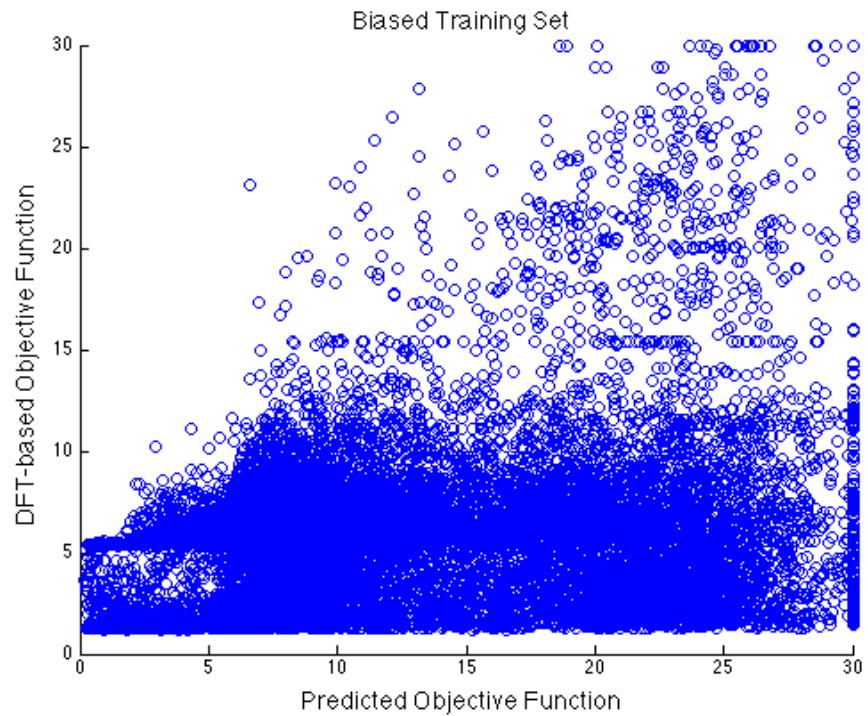
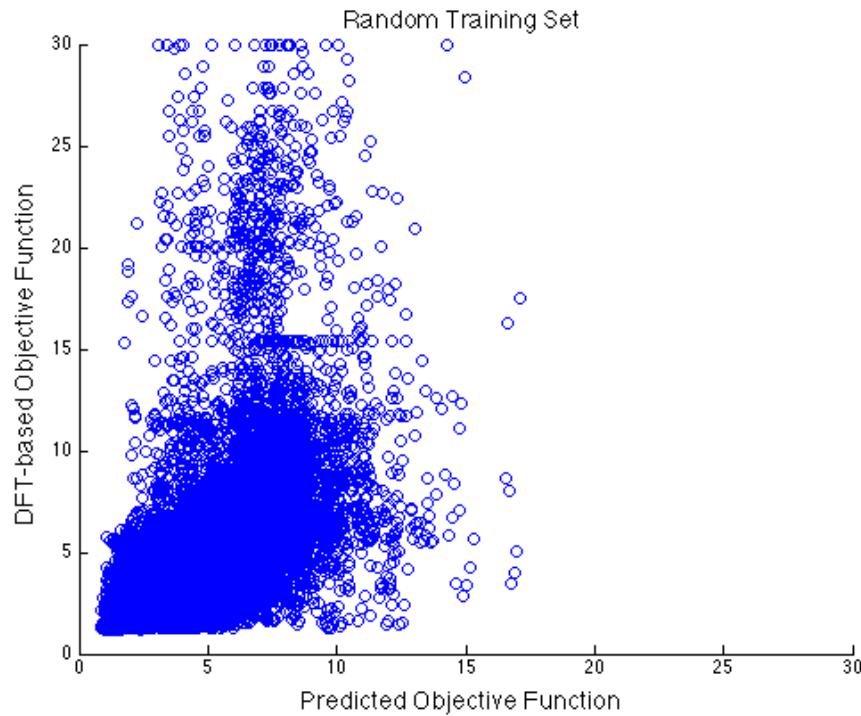


# The Next Demo Step

- Predicting Water Splitting
- Compared to genetic algorithm

Metals ~18000  
Non-metals ~700

Jain, Anubhav, et al. "Performance of genetic algorithms in search for water splitting perovskites." Journal of Materials Science 48.19 (2013): 6519-6534.



# Quick Demo



# Why we should win? Because ...

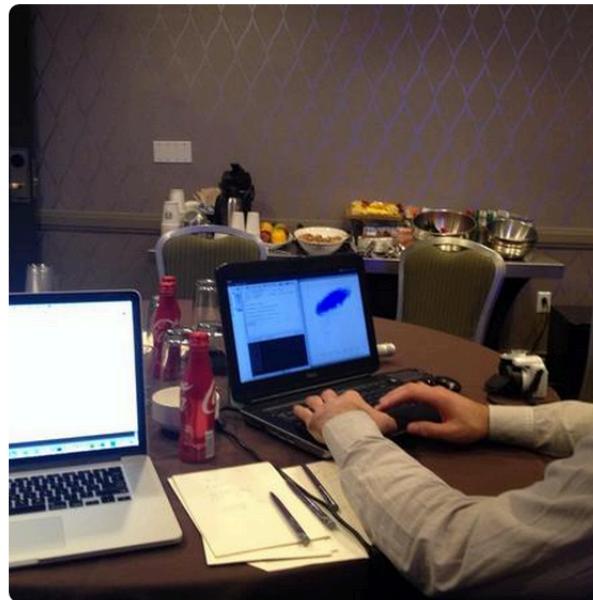


Andrew Long

@awlong89



The last survivors get all the spoils #MatHack  
#f14mrs



3:38 AM - 3 Dec 2014

A photograph of two men smiling at the camera. The man on the left is wearing a dark suit jacket over a light-colored shirt and has a lanyard with a badge that says "WELCOME". The man on the right has a beard and is wearing a dark zip-up hoodie. They appear to be at a conference or event.

Thanks for hosting  
MatHack 2014!