Python Project MSE 110

William Cook

First Prompt - 1.1

Oxide vs. Nitride Comparison

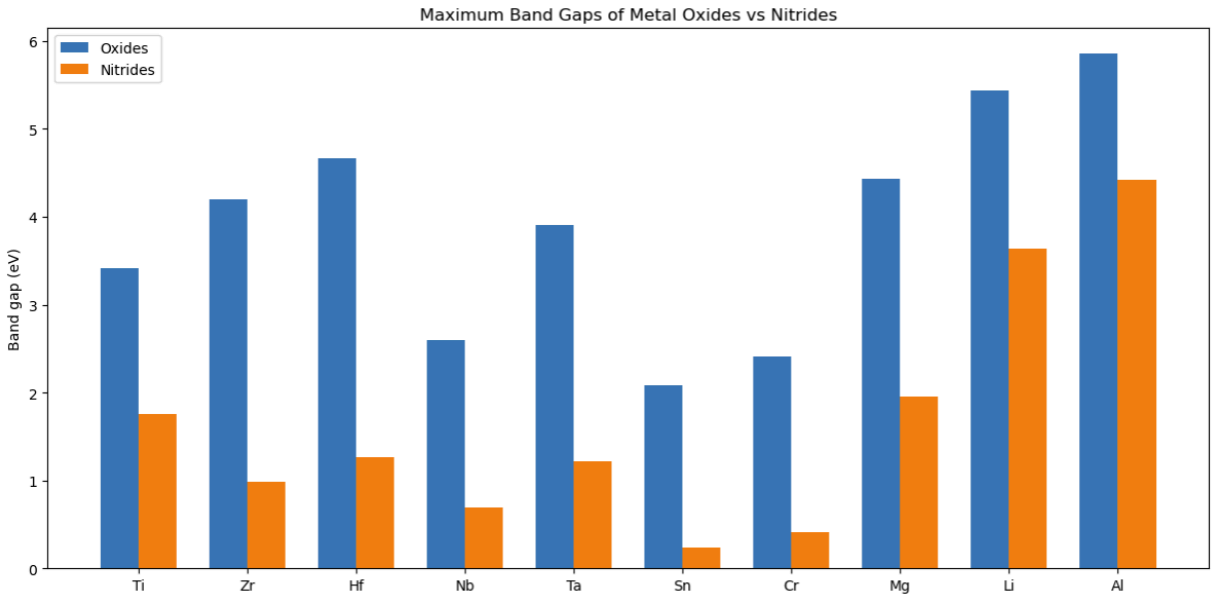
Really simple code, just input 10 metals into the system

Then, it scans for all oxides and nitrides of the metals and ensures a known band gap

Afterward, it will take the MAX band gap and keep it as the variable

Finally, it takes the max band gap and plots it for each metal.

Trends: Oxides seem to have a higher band gap than nitrides, meaning oxides are less conductive than nitrides for most metals. I did test a few outliers, such as Ag, whose nitrides seemed to have a higher band gap than oxides, but for most metals, this trend applies.



Second Prompt - 2.2

Semiconductor Finder

This one takes a user defined chemical system, in which I chose Ti-S

It then scans all materials that contain that chemical system.

It then takes the previously defined definition of semiconductor, which enforces a band gap of 0.1 to 4, and applies it to the materials, filtering them down to just the semiconductors.

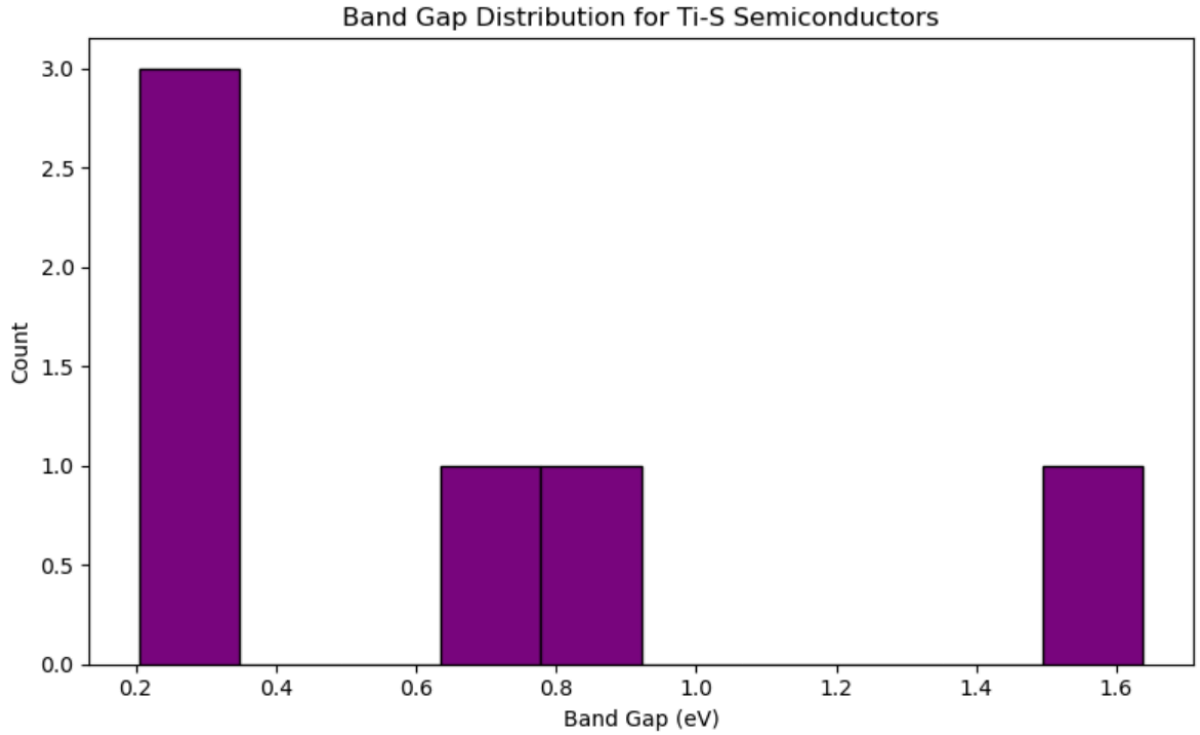
It takes their formation energy if they pass that test, then adds it to a dataframe so it can be graphed.

It first prints out a table of the passing materials with their band gap and their formation energy.

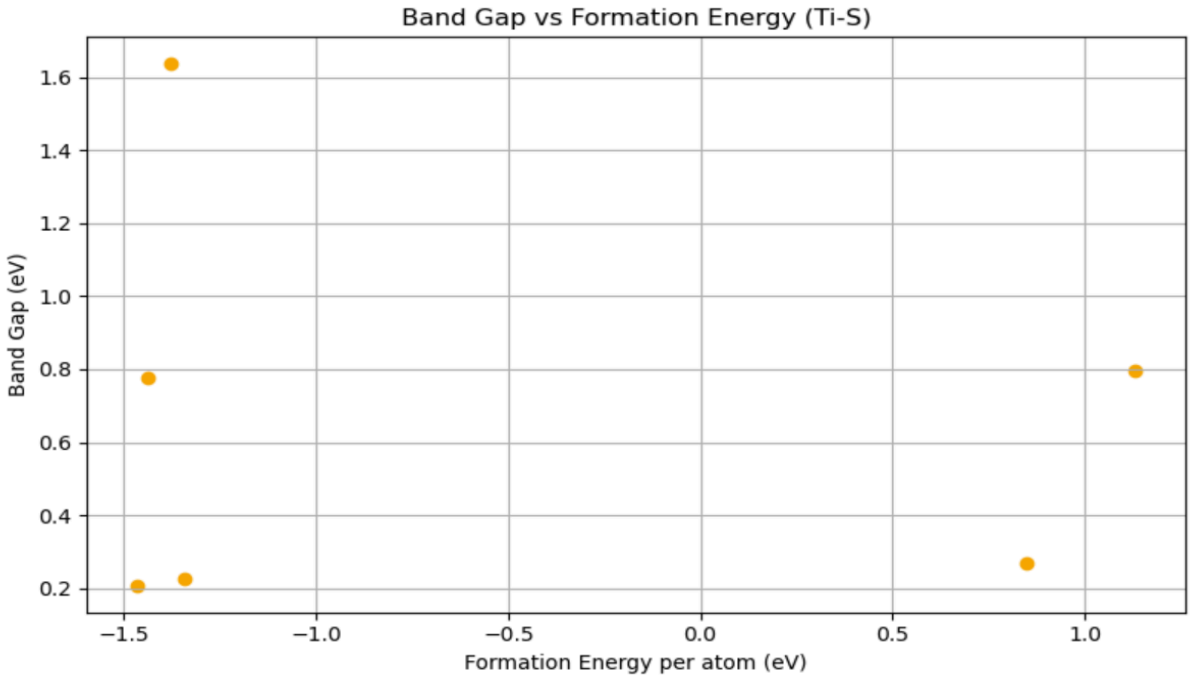
Semiconducting materials in Ti-S:

formula	band_gap (eV)	formation_energy_per_atom (eV)
TiS2	0.2055	-1.465774
TiS3	0.2261	-1.341742
Ti3S4	0.2669	0.847748
TiS2	0.7773	-1.439357
TiS	0.7957	1.132035
TiS2	1.6382	-1.380241

It then forms a bar graph representing the amount of materials that have a specific band gap.



Lastly, it forms a scatter plot of their band gap vs their formation energy.



This results in an easy way to filter materials of a certain criteria in order to find the best semiconductor with the least amount of formation energy.