Project Proposal: Database Screening for Compatible Materials with Wireless Charging

MAY 22, 2019

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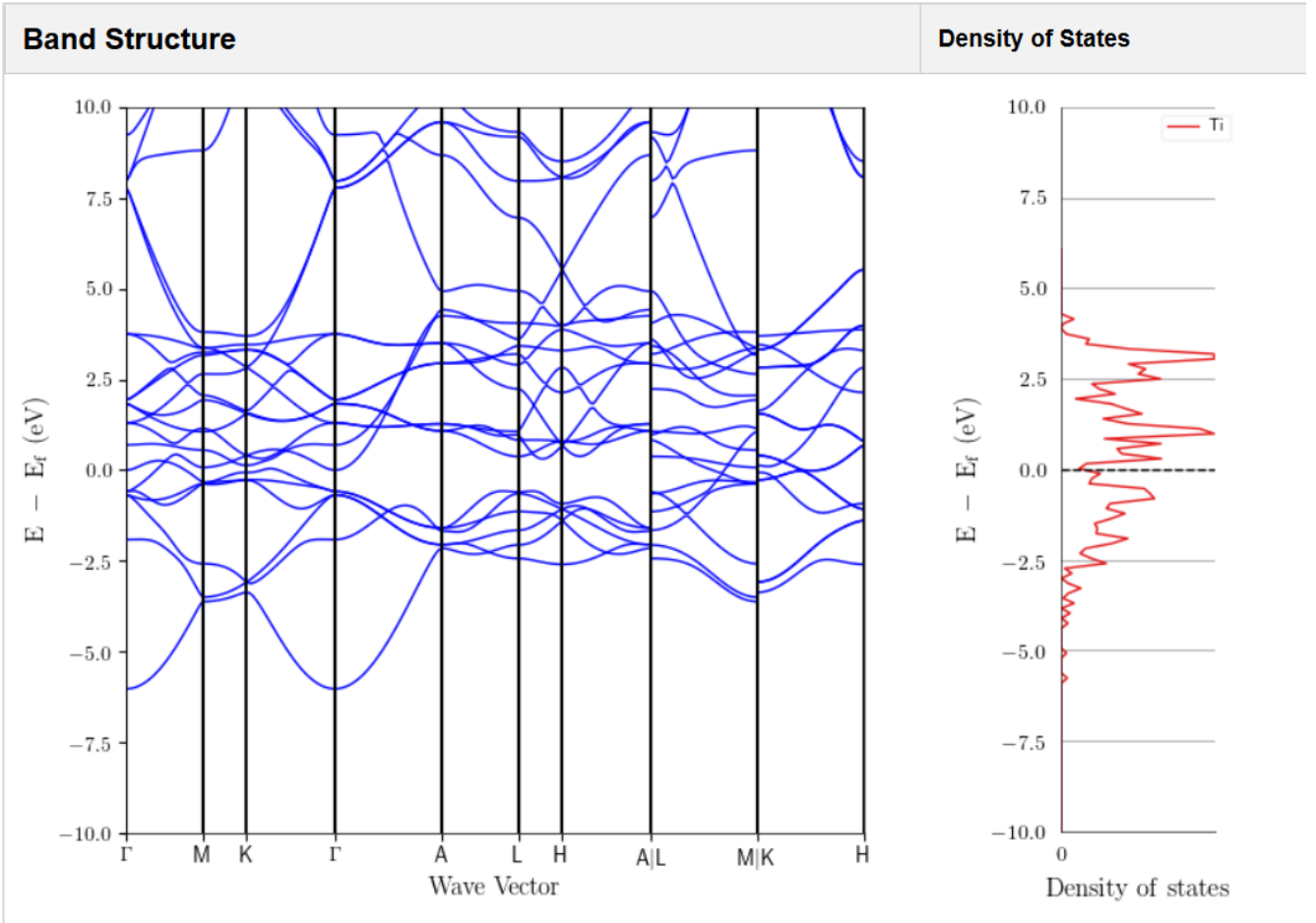
Current problem

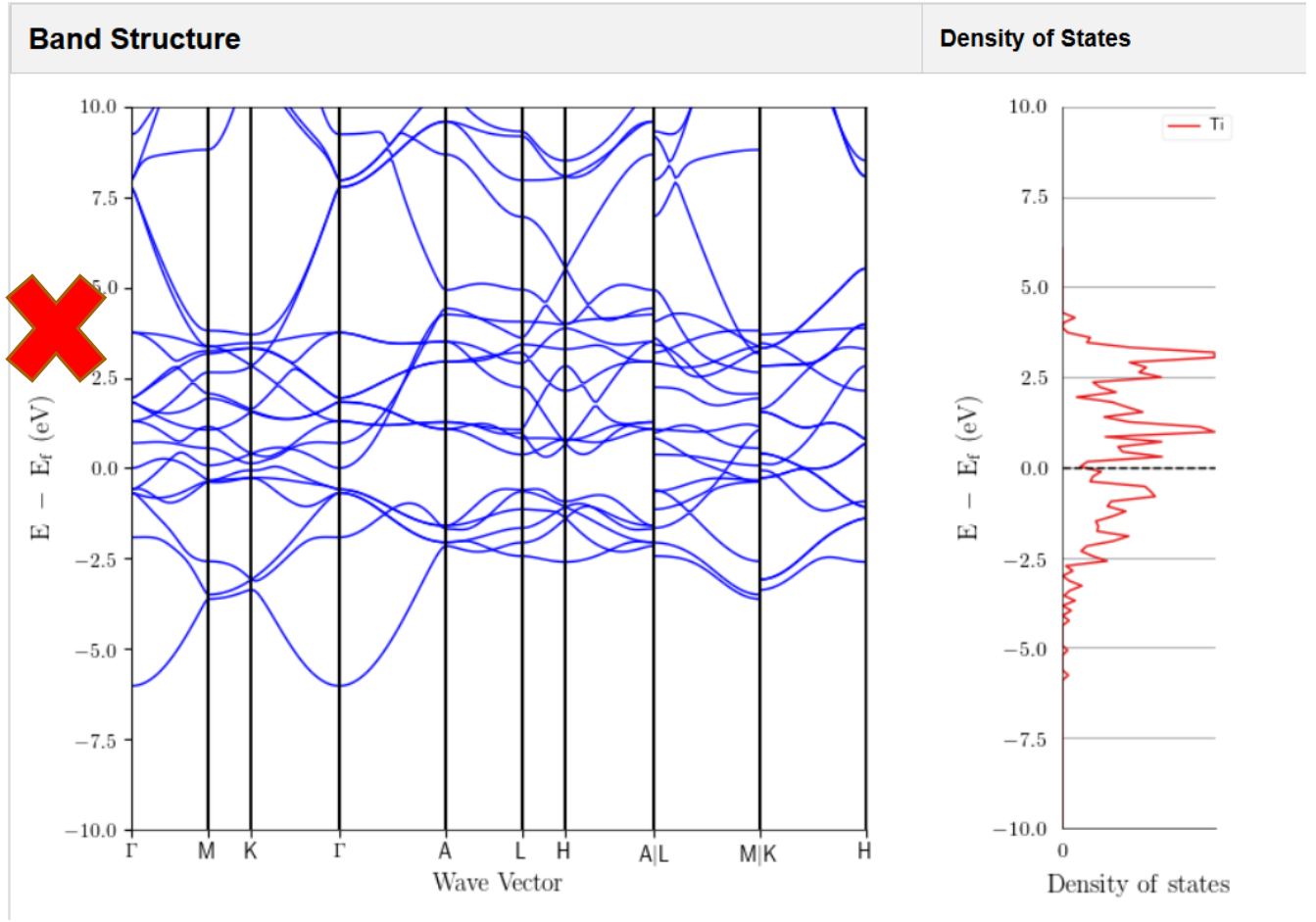
Image taken from: https://www.nbcnews.com/tech/tech-news/don-t-drop-it-shocking-repair-prices-iphone-x-n821071

Why do we use glass? - Titanium



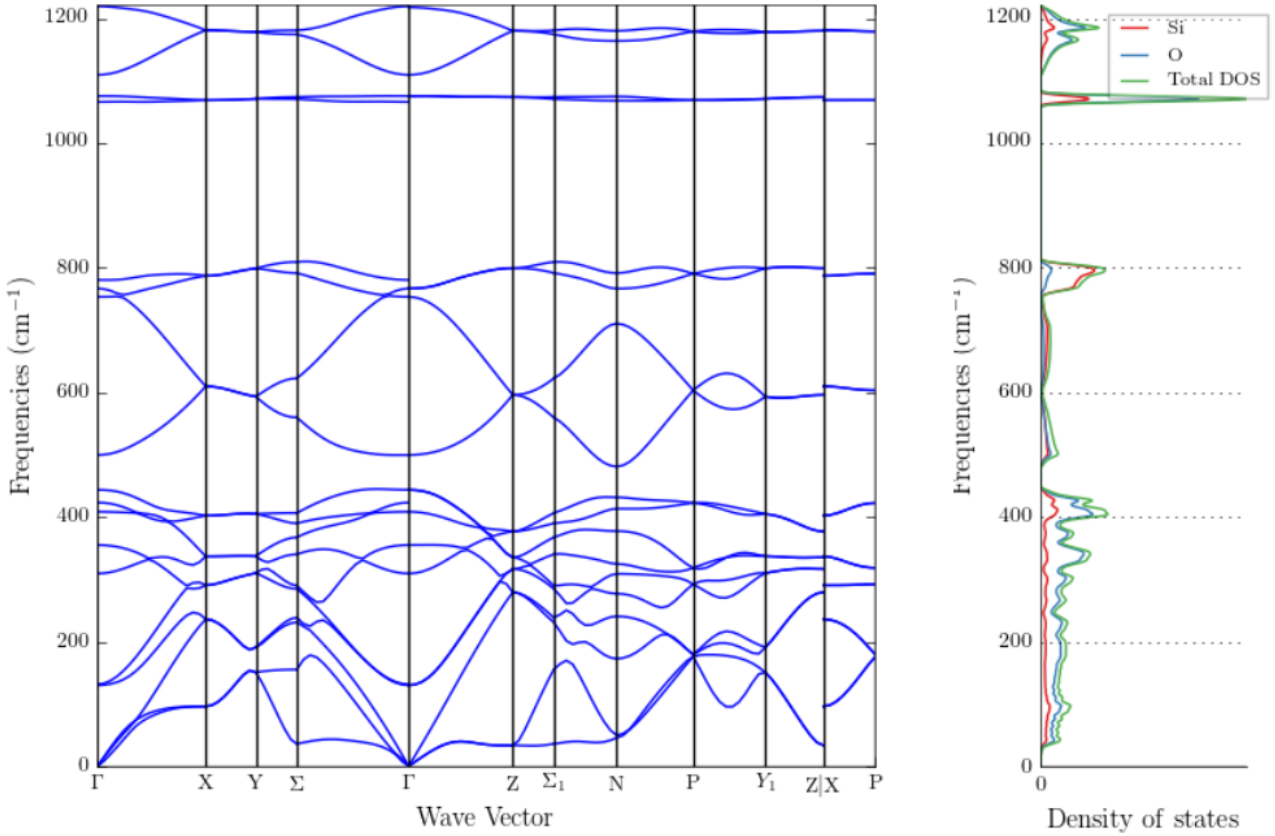
Why do we use glass? - Titanium

Device Charging Electronic Wave

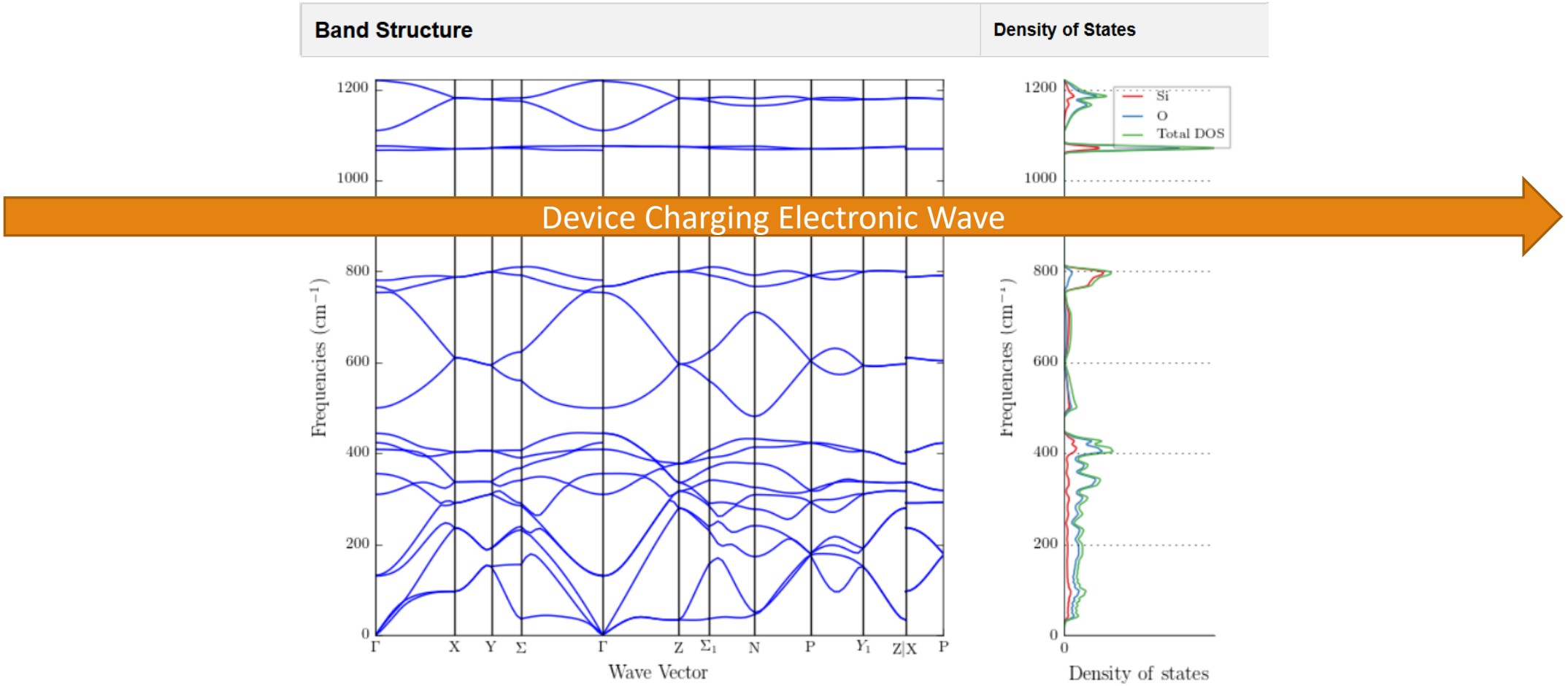


Why do we use glass? - Glass

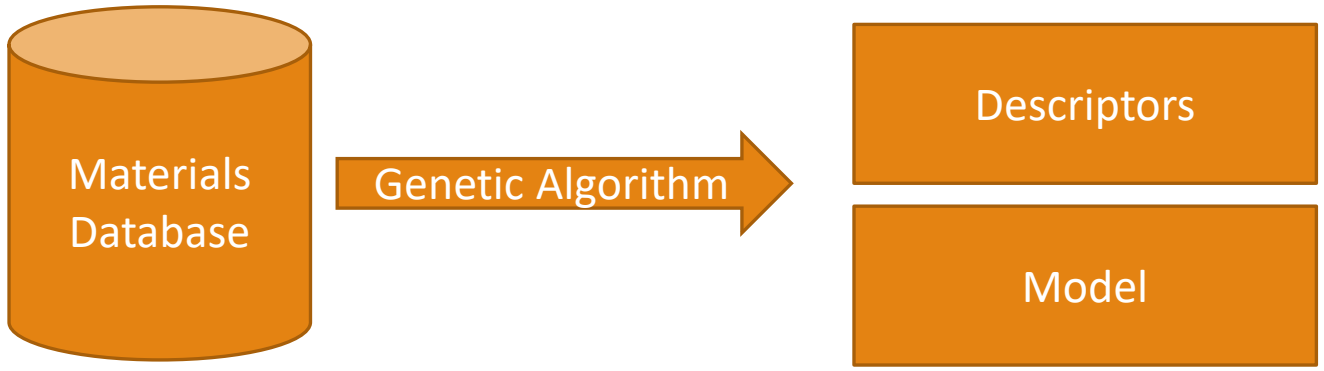
Band Structure	Density of States



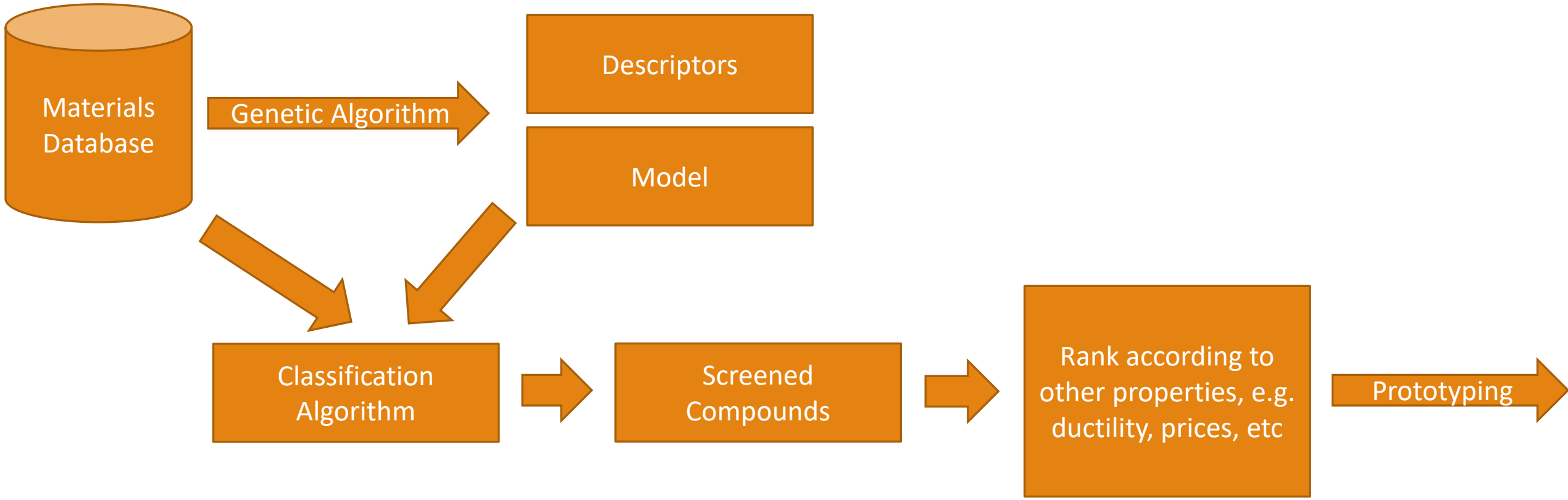
Why do we use glass? - Glass



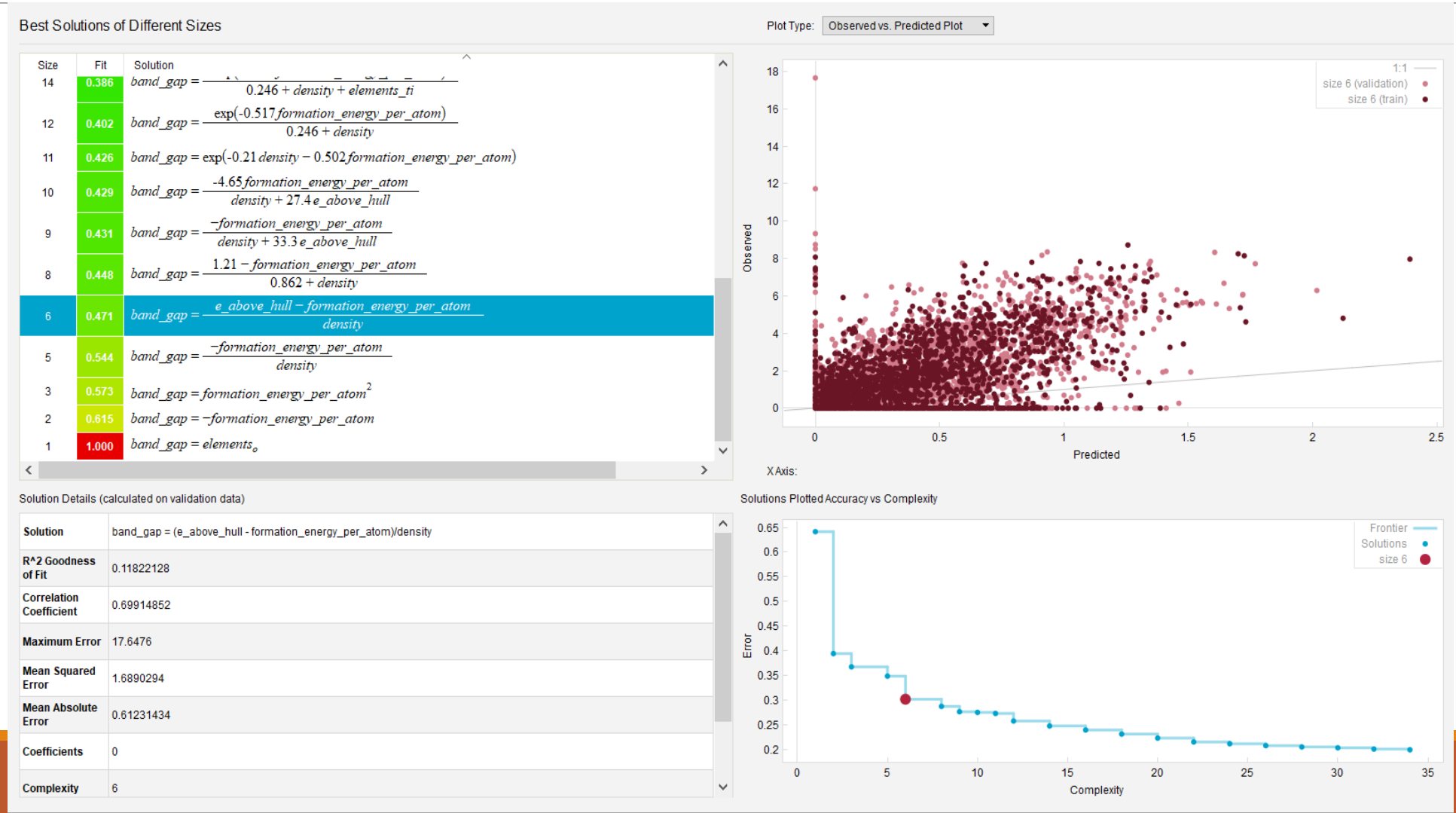
Screening Process



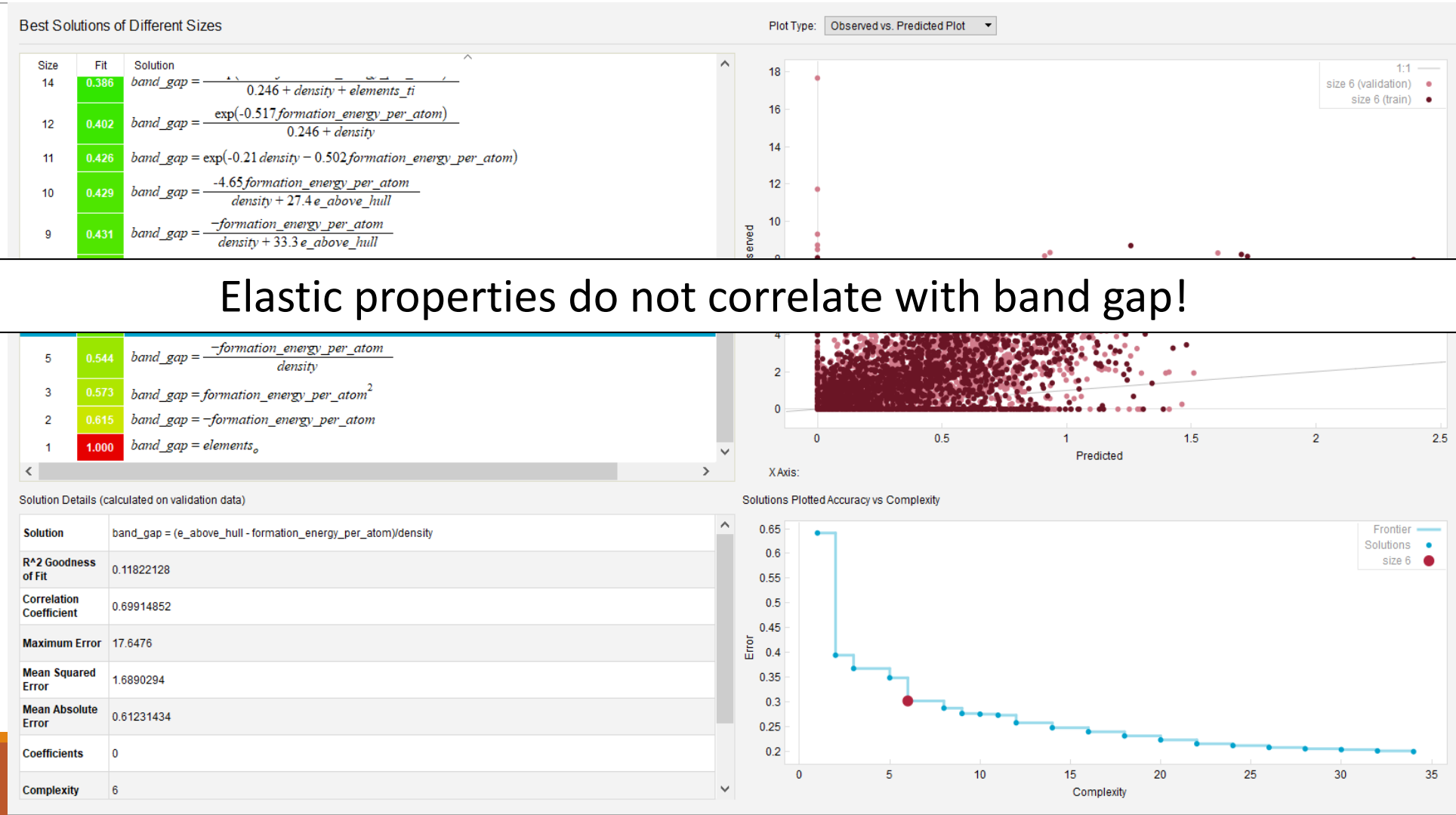
Screening Process



Adding Elastic Properties – 13,321 materials



Adding Elastic Properties – 13,321 materials



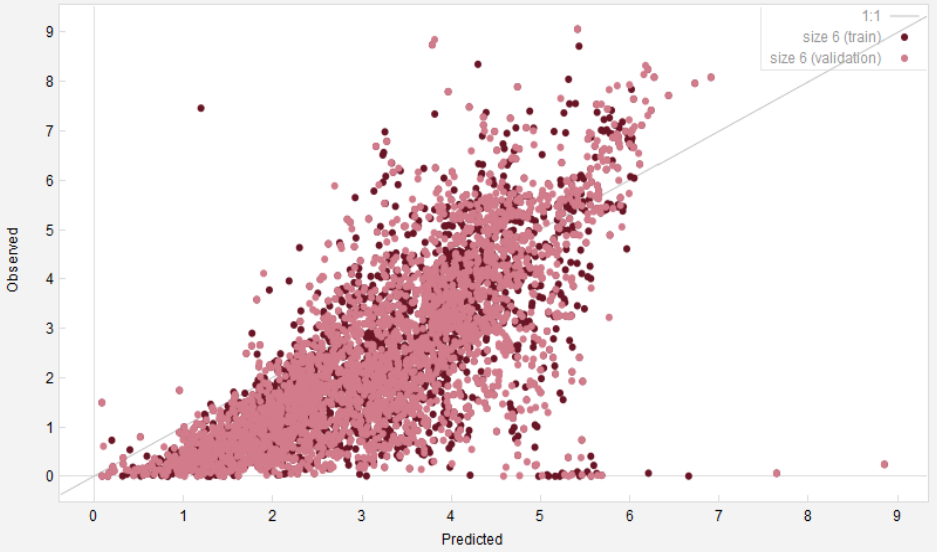
Elastic properties do not correlate with band gap!

Dataset with dielectric properties – 4,724 materials

Best Solutions of Different Sizes

Size	Fit	Solution
16	0.256	$band\_gap = \frac{3.04 + elements_h - formation\_energy\_per\_atom - elements\_mn - elements_v - 0.271}{index\_of\_refraction}$
14	0.268	$band\_gap = \frac{3 + elements_h - formation\_energy\_per\_atom - elements\_mn - 0.255\,density}{index\_of\_refraction}$
12	0.277	$band\_gap = \frac{2.81 + elements_h - formation\_energy\_per\_atom - elements\_mn - elements_v}{index\_of\_refraction}$
10	0.285	$band\_gap = \frac{3.24 + elements_h - formation\_energy\_per\_atom}{index\_of\_refraction} - elements\_mn$
8	0.301	$band\_gap = elements_h + \frac{3.3 - formation\_energy\_per\_atom}{index\_of\_refraction}$
6	0.339	$band\_gap = \frac{4.72 - formation\_energy\_per\_atom}{index\_of\_refraction}$
4	0.423	$band\_gap = \frac{5.61}{index\_of\_refraction}$
3	0.534	$band\_gap = elements_h - formation\_energy\_per\_atom$
2	0.642	$band\_gap = -formation\_energy\_per\_atom$
1	1.000	$band\_gap = elements_h$

Plot Type: Observed vs. Predicted Plot

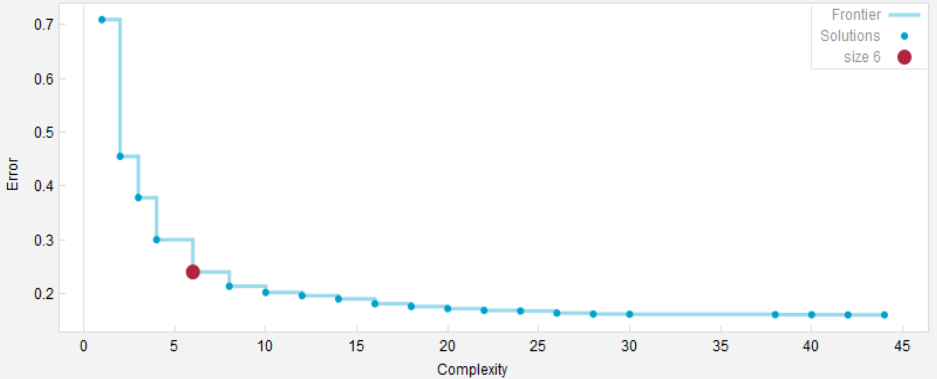


X Axis:

Solution Details (calculated on validation data)

Solution	band_gap = (4.718 - formation_energy_per_atom)/index_of_refraction
R^2 Goodness of Fit	0.40262443
Correlation Coefficient	0.76508197
Maximum Error	8.6101291
Mean Squared Error	1.8486592
Mean Absolute Error	1.0796188
Coefficients	1
Complexity	6

Solutions Plotted Accuracy vs Complexity



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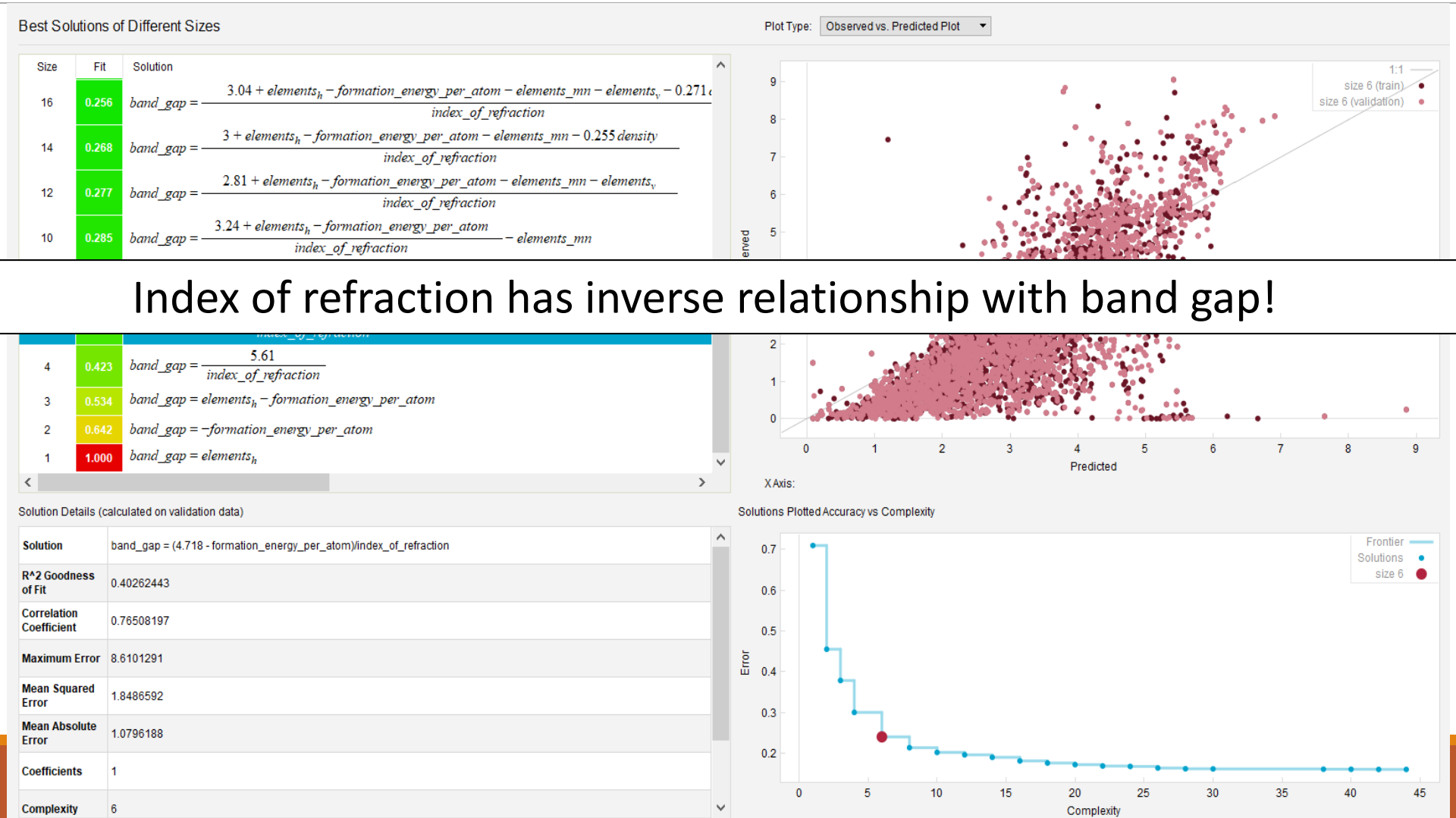

Index of refraction has inverse relationship with band gap!

Takeaways

1. To make wireless charging realize its potential, a resilient material that works with it is a must.
2. Metals in general are resilient, but reflect the charging waves.
3. Glass works, but is brittle.
4. Screening materials database will pre-screen materials for prototyping.
5. After adding mechanical properties to the original 13,321 data set, increasing the file size by a factor of 10, I found that mechanical properties do not correlate to band gap, this validates the chosen screening steps.
6. The existence of oxygen and hydrogen indicates band gap
7. On top of the recently found inverse relation to density, and screening 4,724 materials with dielectric properties found that index of refraction are also inversely proportional to band gap.