

Project Proposal: Database Screening for Compatible Materials with Wireless Charging

MAY 22, 2019

PANDU WISESA

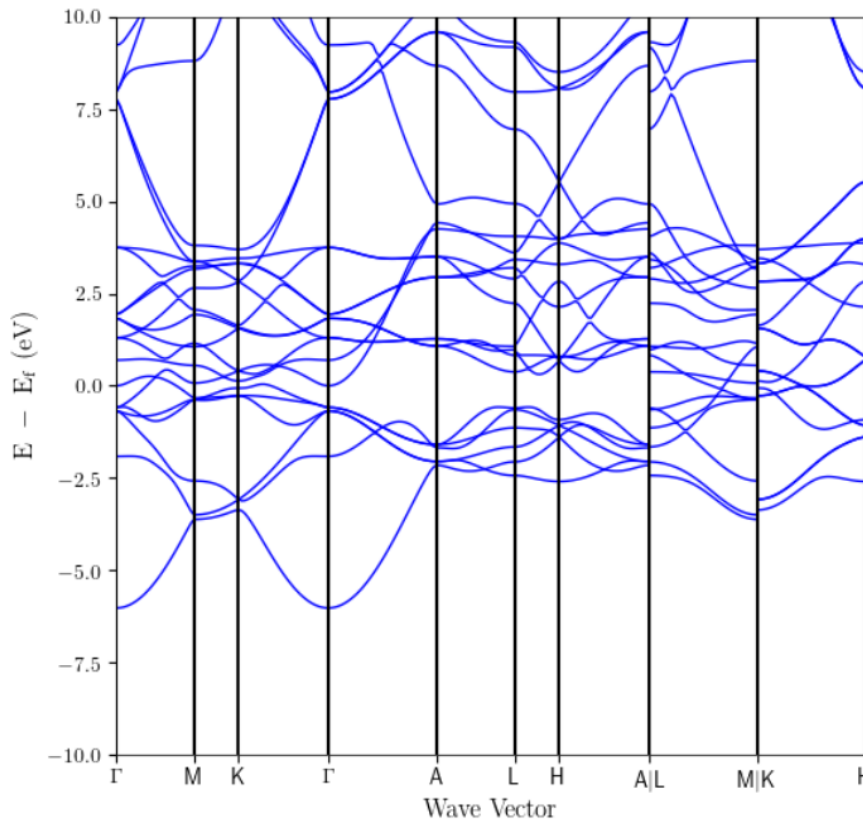


Current problem

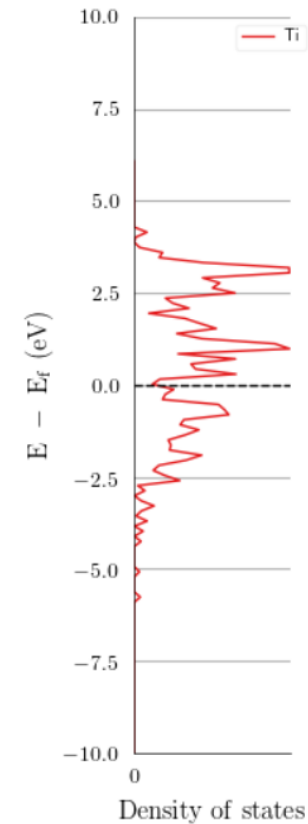


Why do we use glass? - Titanium

Band Structure

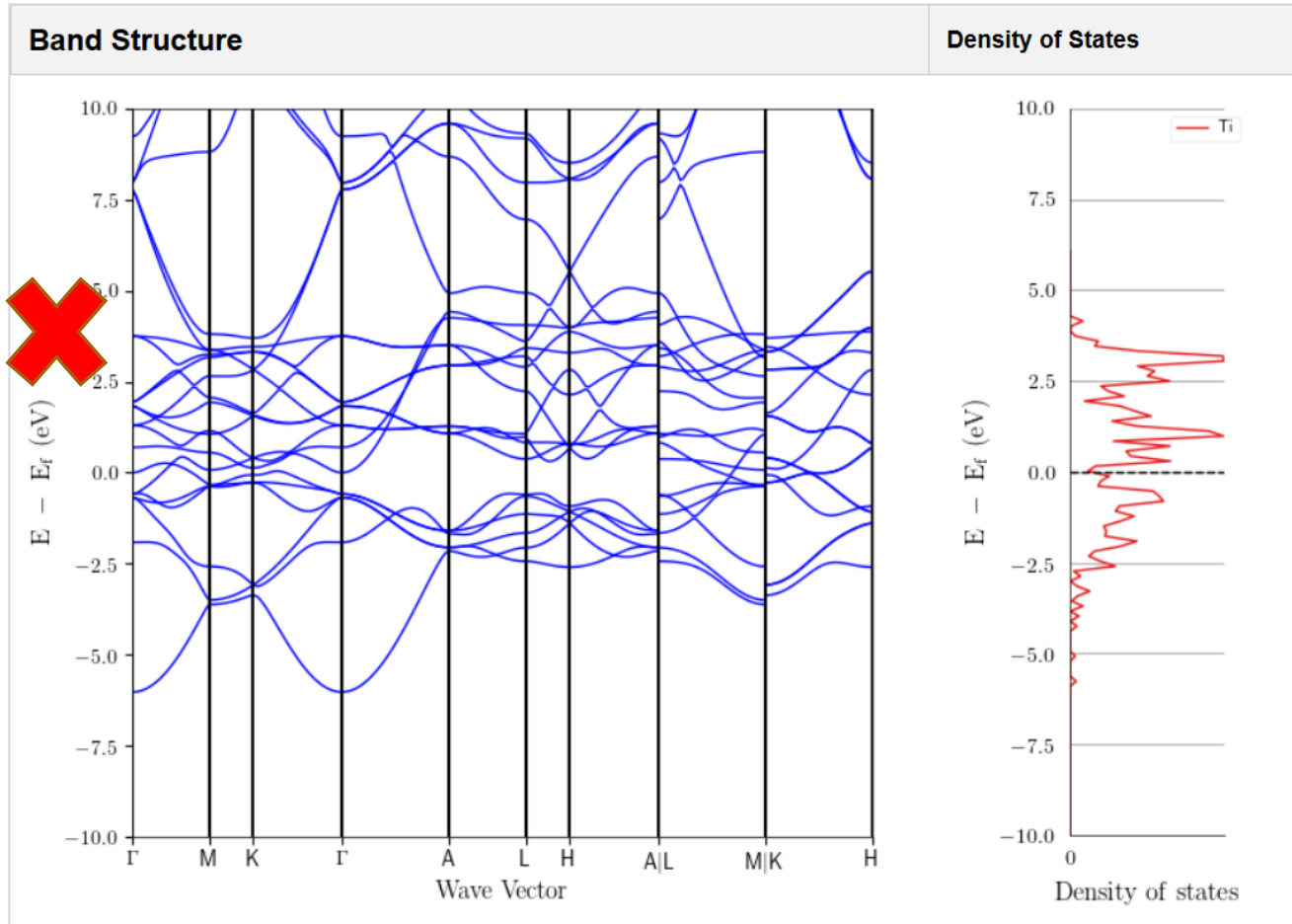


Density of States



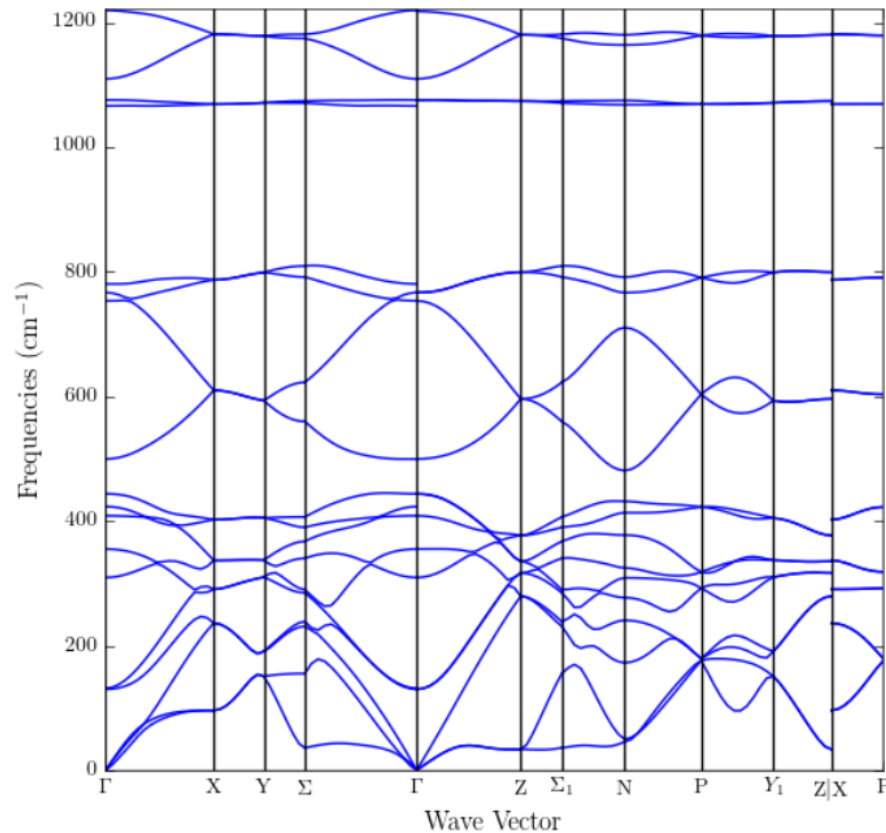
Why do we use glass? - Titanium

Device Charging
Electronic Wave

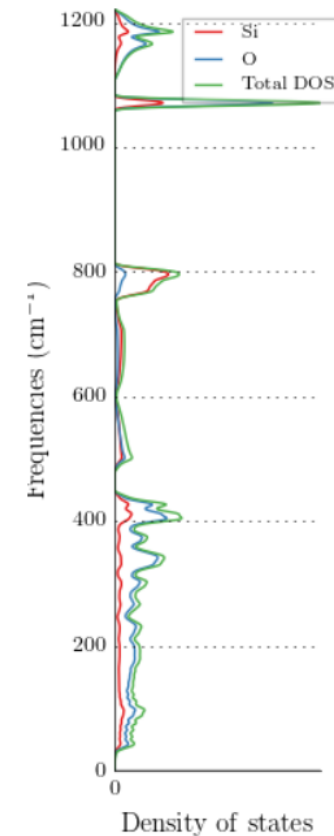


Why do we use glass? - Glass

Band Structure

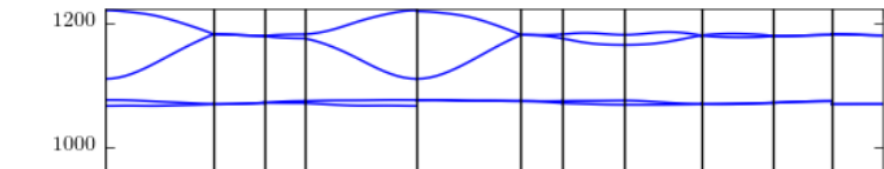


Density of States

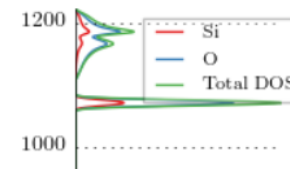


Why do we use glass? - Glass

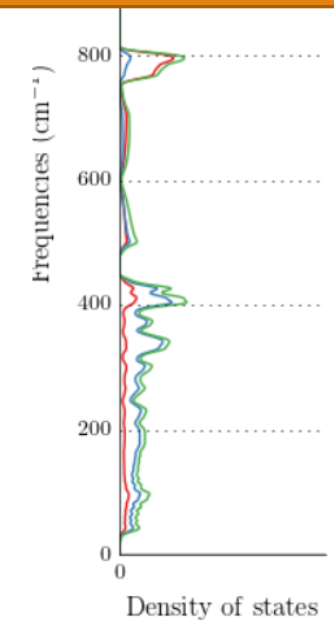
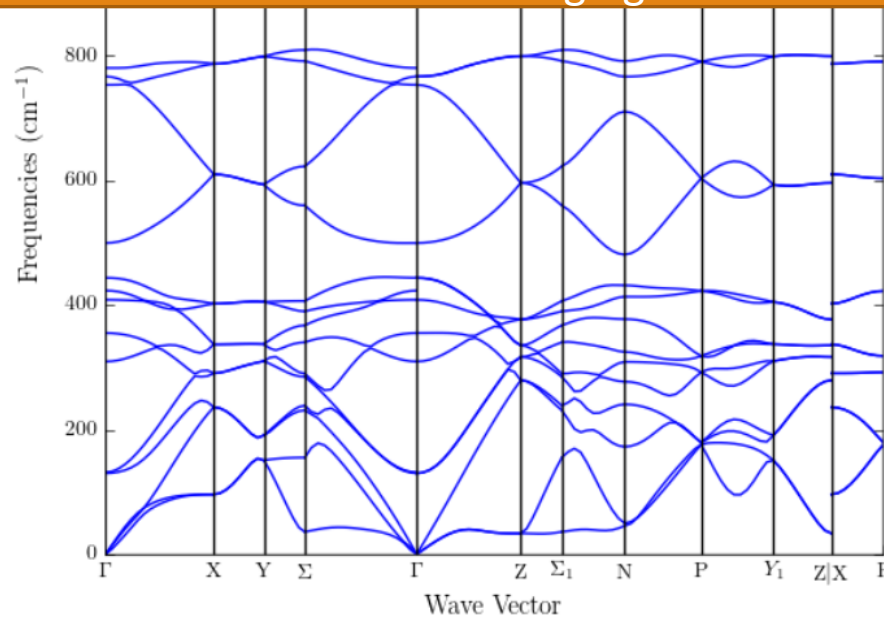
Band Structure



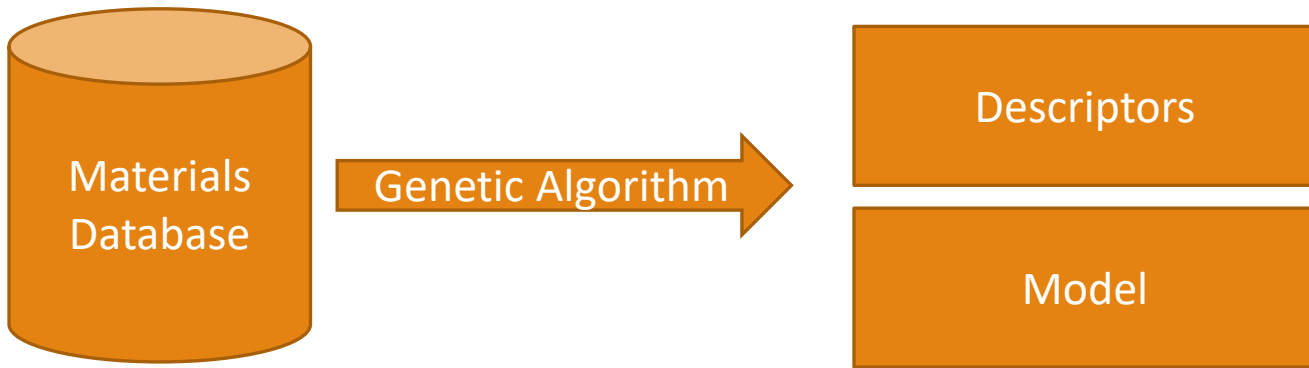
Density of States



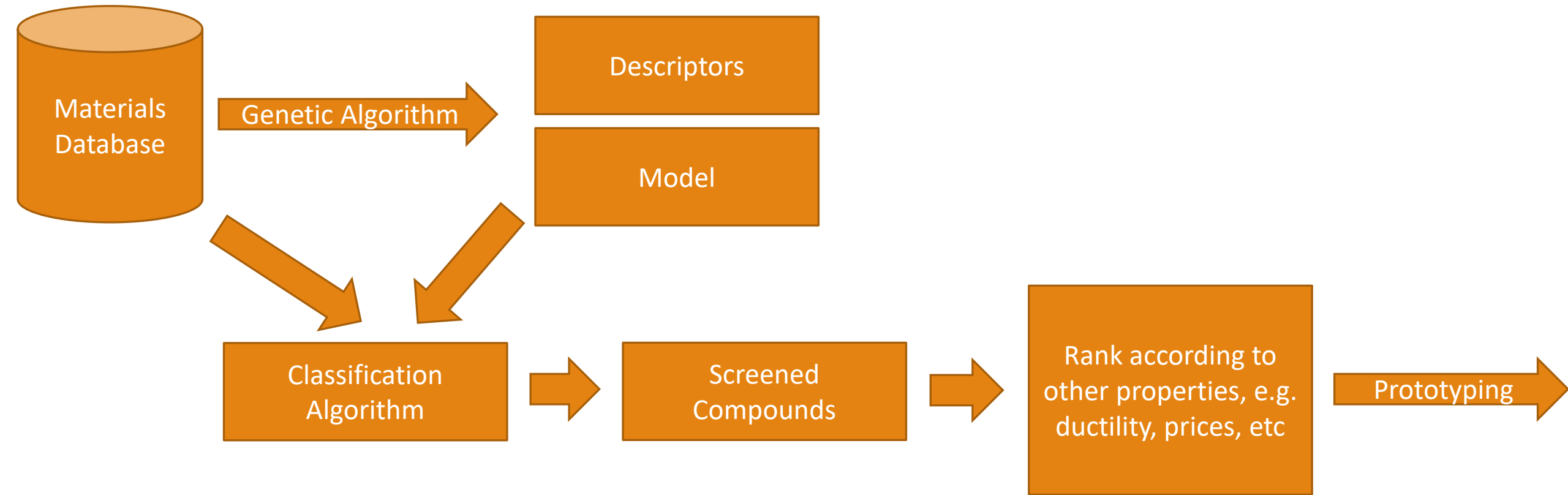
Device Charging Electronic Wave



Screening Process



Screening Process



Adding Elastic Properties

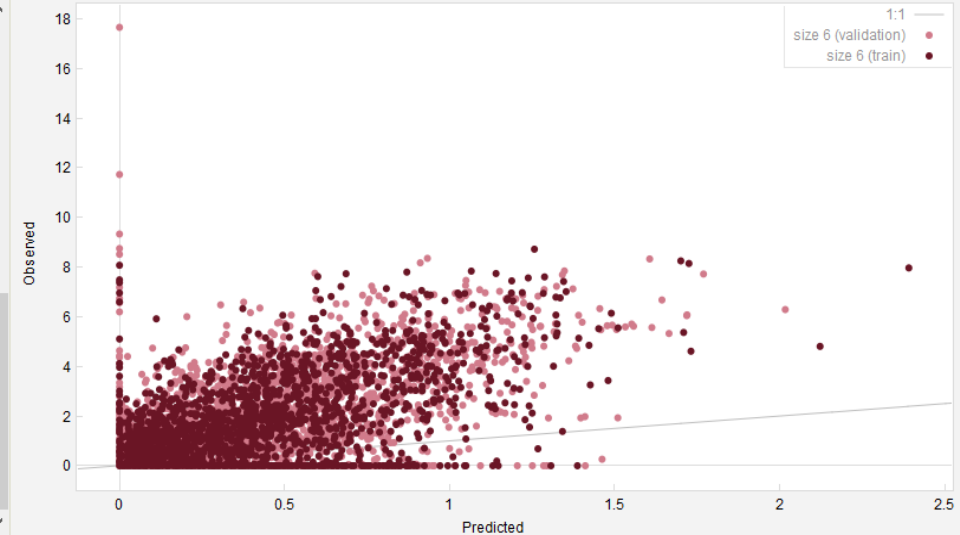
Best Solutions of Different Sizes

Size	Fit	Solution
14	0.386	$\text{band_gap} = \frac{0.246 + \text{density} + \text{elements_fi}}{0.246 + \text{density}}$
12	0.402	$\text{band_gap} = \frac{\exp(-0.517 \text{formation_energy_per_atom})}{0.246 + \text{density}}$
11	0.426	$\text{band_gap} = \exp(-0.21 \text{density} - 0.502 \text{formation_energy_per_atom})$
10	0.429	$\text{band_gap} = \frac{-4.65 \text{formation_energy_per_atom}}{\text{density} + 27.4 e_above_hull}$
9	0.431	$\text{band_gap} = \frac{-\text{formation_energy_per_atom}}{\text{density} + 33.3 e_above_hull}$
8	0.448	$\text{band_gap} = \frac{1.21 - \text{formation_energy_per_atom}}{0.862 + \text{density}}$
6	0.471	$\text{band_gap} = \frac{e_above_hull - \text{formation_energy_per_atom}}{\text{density}}$
5	0.544	$\text{band_gap} = \frac{-\text{formation_energy_per_atom}}{\text{density}}$
3	0.573	$\text{band_gap} = \text{formation_energy_per_atom}^2$
2	0.615	$\text{band_gap} = -\text{formation_energy_per_atom}$
1	1.000	$\text{band_gap} = \text{elements}_o$

Solution Details (calculated on validation data)

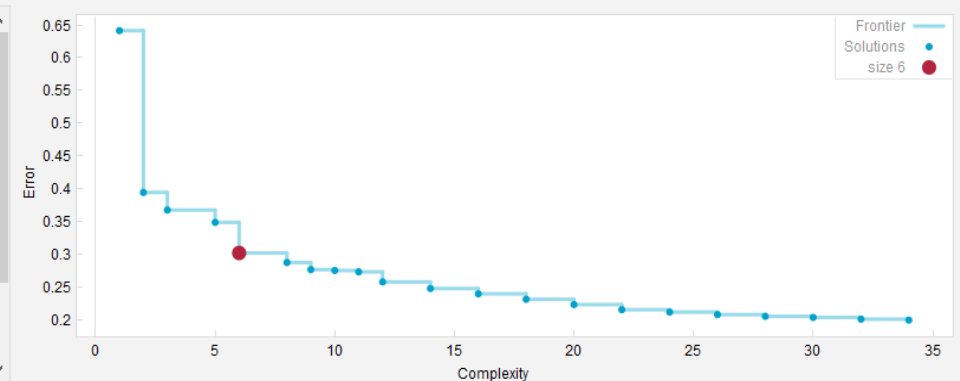
Solution	$\text{band_gap} = (e_above_hull - \text{formation_energy_per_atom}) / \text{density}$
R^2 Goodness of Fit	0.11822128
Correlation Coefficient	0.69914852
Maximum Error	17.6476
Mean Squared Error	1.6890294
Mean Absolute Error	0.61231434
Coefficients	0
Complexity	6

Plot Type: Observed vs. Predicted Plot

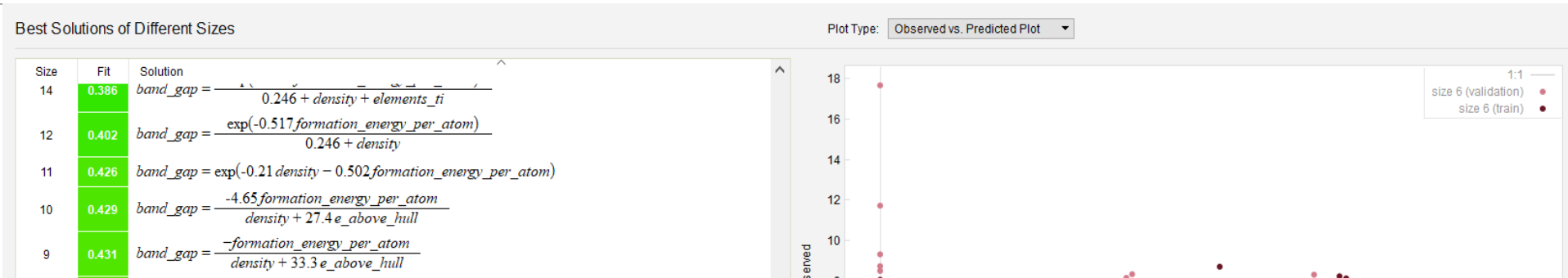


X Axis:

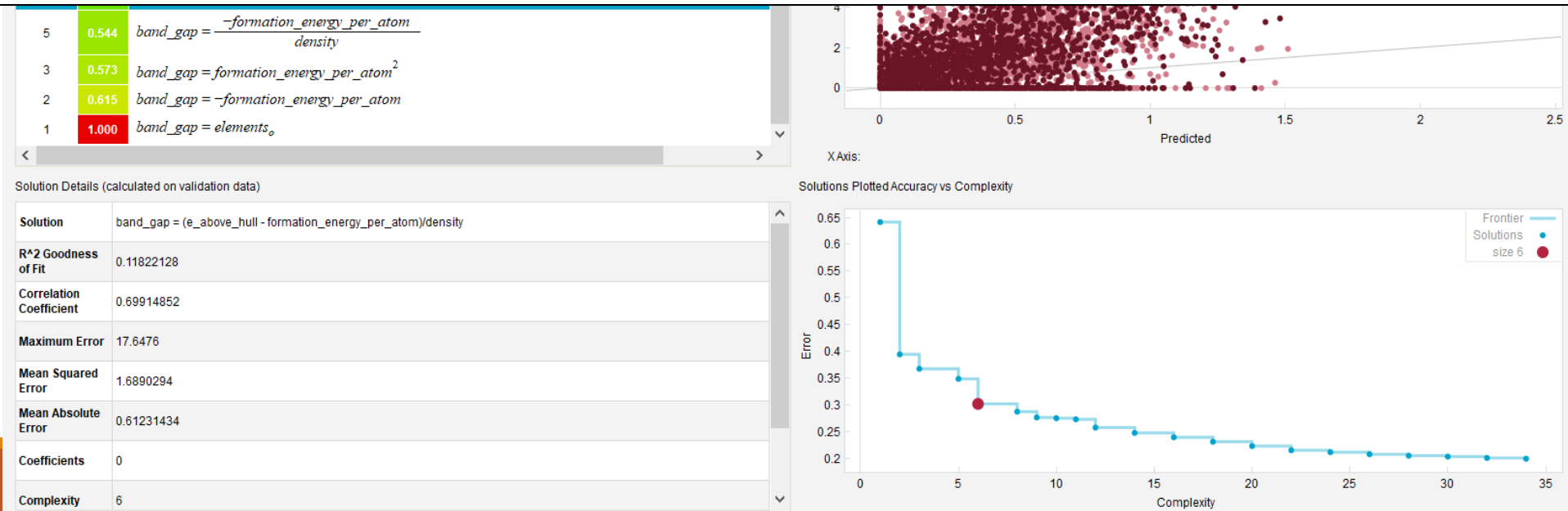
Solutions Plotted Accuracy vs Complexity



Adding Elastic Properties



Elastic properties do not correlate with band gap!



Dataset with dielectric properties

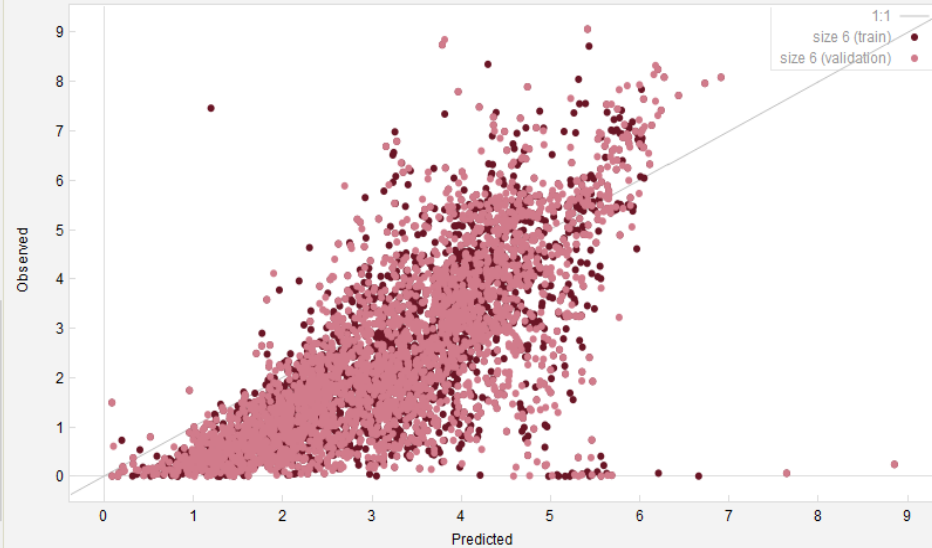
Best Solutions of Different Sizes

Size	Fit	Solution
16	0.256	$\text{band_gap} = \frac{3.04 + \text{elements}_h - \text{formation_energy_per_atom} - \text{elements_mn} - \text{elements}_v - 0.271}{\text{index_of_refraction}}$
14	0.268	$\text{band_gap} = \frac{3 + \text{elements}_h - \text{formation_energy_per_atom} - \text{elements_mn} - 0.255 \text{ density}}{\text{index_of_refraction}}$
12	0.277	$\text{band_gap} = \frac{2.81 + \text{elements}_h - \text{formation_energy_per_atom} - \text{elements_mn} - \text{elements}_v}{\text{index_of_refraction}}$
10	0.285	$\text{band_gap} = \frac{3.24 + \text{elements}_h - \text{formation_energy_per_atom}}{\text{index_of_refraction}} - \text{elements_mn}$
8	0.301	$\text{band_gap} = \text{elements}_h + \frac{3.3 - \text{formation_energy_per_atom}}{\text{index_of_refraction}}$
6	0.339	$\text{band_gap} = \frac{4.72 - \text{formation_energy_per_atom}}{\text{index_of_refraction}}$
4	0.423	$\text{band_gap} = \frac{5.61}{\text{index_of_refraction}}$
3	0.534	$\text{band_gap} = \text{elements}_h - \text{formation_energy_per_atom}$
2	0.642	$\text{band_gap} = -\text{formation_energy_per_atom}$
1	1.000	$\text{band_gap} = \text{elements}_h$

Solution Details (calculated on validation data)

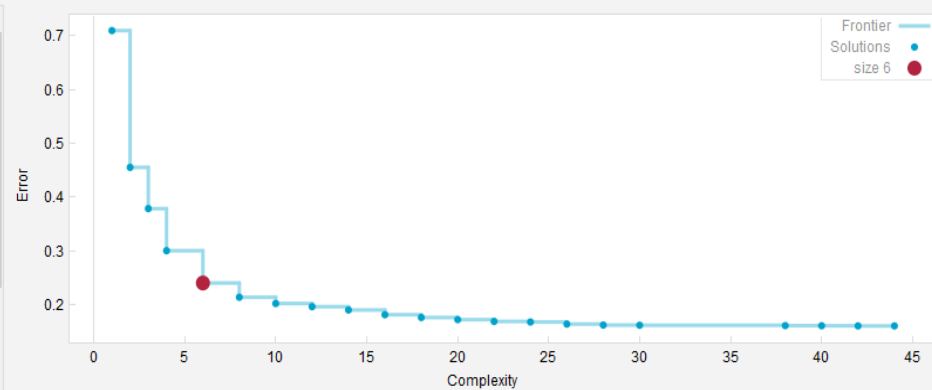
Solution	$\text{band_gap} = (4.718 - \text{formation_energy_per_atom}) / \text{index_of_refraction}$
R ² Goodness of Fit	0.40262443
Correlation Coefficient	0.76508197
Maximum Error	8.6101291
Mean Squared Error	1.8486592
Mean Absolute Error	1.0796188
Coefficients	1
Complexity	6

Plot Type: Observed vs. Predicted Plot

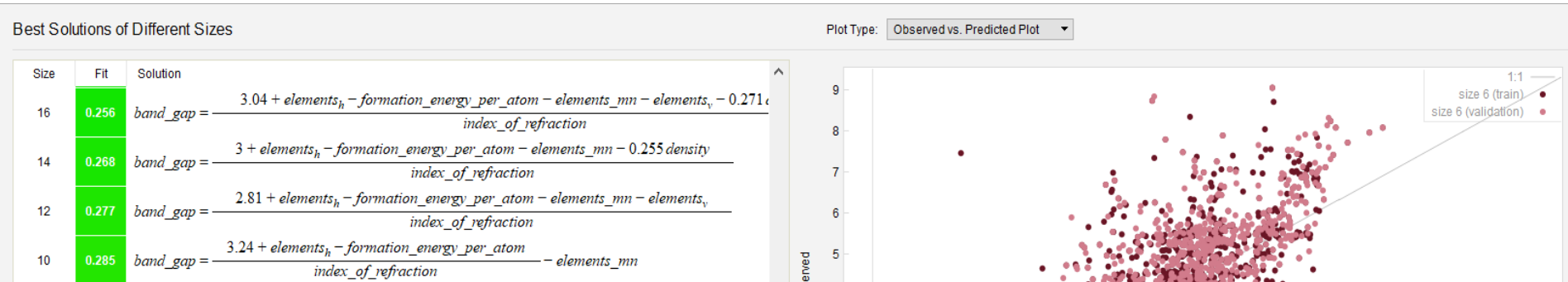


X Axis:

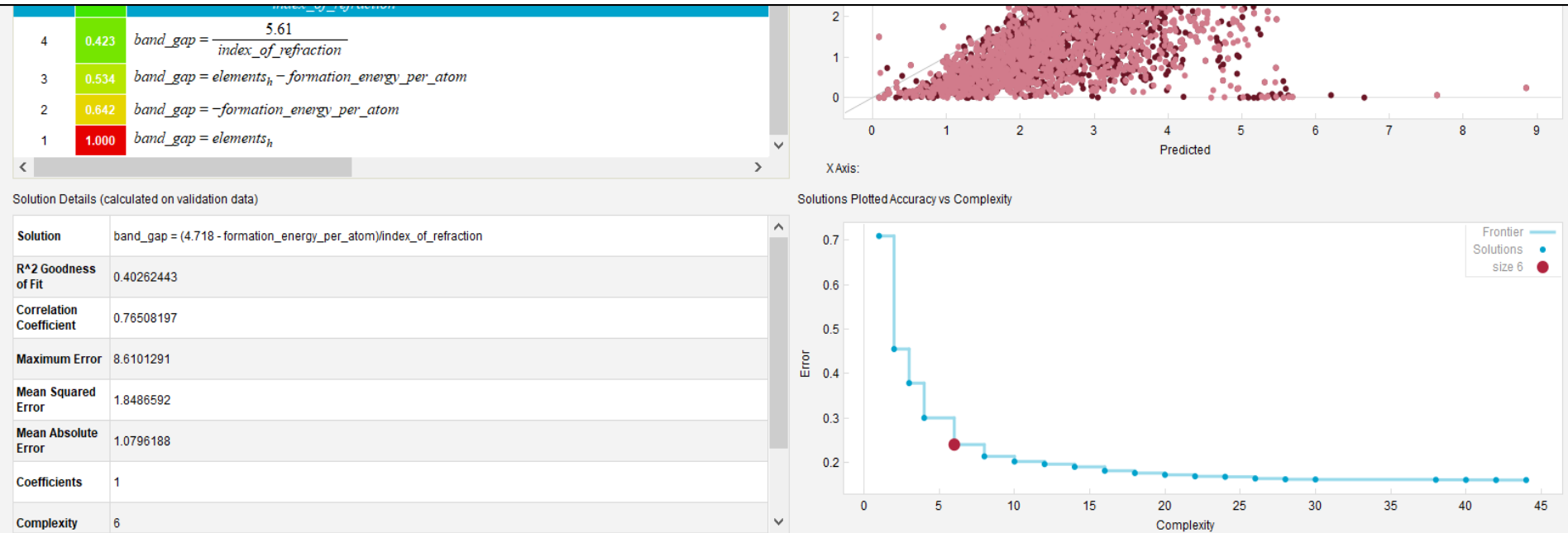
Solutions Plotted Accuracy vs Complexity



Dataset with dielectric properties



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. Mechanical properties do not correlate to band gap
6. The existence of oxygen and hydrogen indicates band gap
7. Density and index of refraction are inversely proportional to band gap.