

DATA VISUALISATION

(CSE3020 - L43+L44)

EMBEDDED PROJECT

FALL SEMESTER 2021-22

A critical study of properties affecting the critical temperature of a superconductor: Visualization and analysis of their trends and variations

FINAL REPORT

GROUP 23

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REVIEW 1

■ DATASET DETAILS

The dataset was downloaded from the UCI Machine Learning Repository:
<https://archive.ics.uci.edu/ml/datasets/Superconductivity+Data>.

It is sourced from: *Hamidieh, Kam, A data-driven statistical model for predicting the critical temperature of a superconductor, Computational Materials Science, Volume 154, November 2018, Pages 346-354.*

The dataset consists of 2 CSV files: **train.csv** and **unique_m.csv**. The first file: **train.csv** contains the data related to the physical and chemical properties of the superconductor materials. The second file: **unique_m.csv** contains the chemical formulae of the superconducting materials, and also the element-wise stoichiometric composition of each material.

In **train.csv**: 81 attributes and 21263 rows/instances

In **unique_m.csv**: 88 attributes and 21263 rows

We now describe our implemented dataset.

The different attributes described are:

In train.csv:

1. Number of constituent elements in the material
2. 8 primary attributes: chemical/physical properties of each superconducting material
 - Atomic mass, first ionization enthalpy, atomic radius, density, electron affinity, fusion heat, thermal conductivity, valence.
 - a. For each primary attribute there are 10 derived attributes:
 - i. Mean
 - ii. Weighted mean
 - iii. Geometric mean
 - iv. Weighted geometric mean
 - v. Entropy
 - vi. Weighted entropy
 - vii. Range
 - viii. Weighted range
 - ix. Standard deviation
 - x. Weighted standard deviation
3. Critical temperature of the superconducting material

The reason these derived attributes are chosen, is because, in chemistry, sometimes a derived form of the primary property has been known to show a better correlation with the target.

We test out the correlation of each derived attribute, and choose the best fit and discard the rest during our analysis.

Note that: t_i = variable under investigation

$$w_i = \frac{t_i}{\sum t_i} = \text{Fraction composition}$$

$$p_i = \text{Stoichiometric fraction, i.e. in } H_2O, p_i \text{ for } H = \frac{2}{3}$$

$$A_i = \frac{p_i w_i}{\sum p_i w_i}$$

The derived attributes are calculated using the following formulae:

Derived attribute	Formula
Mean	$\mu = \frac{t_i}{n}$
Weighted mean	$v = \sum p_i t_i$
Geometric mean	$\sqrt[n]{\prod t_i}$
Weighted geometric mean	$\prod t_i^{p_i}$
Entropy (measure of randomness of the attribute)	$-\sum w_i \ln(w_i)$
Weighted entropy	$-\sum A_i \ln(A_i)$
Range (span of the values of attribute in the constituents)	$\max(t_i - t_j), \quad i, j \in 1, 2, \dots, n$
Weighted range	$\max(p_i t_i - p_j t_j), \quad i, j \in 1, 2, \dots, n$
Standard deviation	$\sqrt{\frac{1}{2} \sum (t_i - \mu)^2}$
Weighted standard deviation	$\sqrt{\sum p_i (t_i - v)^2}$

In unique_m.csv:

1. Stoichiometric coefficient of each element in the chemical formula of the superconducting material (86 rows, from Hydrogen to Radon)
2. Critical temperature of the superconducting material – this common attribute between the two separate files helps us link and cross-reference data between them
3. Chemical formula of the compound

■ DATA ABSTRACTION

1. Attributes in **train.csv**: All attributes are of quantitative type.

number_of_elements	int64
mean_atomic_mass	float64
wtd_mean_atomic_mass	float64
gmean_atomic_mass	float64
wtd_gmean_atomic_mass	float64
entropy_atomic_mass	float64
wtd_entropy_atomic_mass	float64
range_atomic_mass	float64
wtd_range_atomic_mass	float64
std_atomic_mass	float64
wtd_std_atomic_mass	float64
mean_fie	float64
wtd_mean_fie	float64
gmean_fie	float64
wtd_gmean_fie	float64
entropy_fie	float64
wtd_entropy_fie	float64
range_fie	float64
wtd_range_fie	float64
std_fie	float64
wtd_std_fie	float64
mean_atomic_radius	float64
wtd_mean_atomic_radius	float64
gmean_atomic_radius	float64
wtd_gmean_atomic_radius	float64
entropy_atomic_radius	float64
wtd_entropy_atomic_radius	float64
range_atomic_radius	int64
wtd_range_atomic_radius	float64
std_atomic_radius	float64
wtd_std_atomic_radius	float64
mean_Density	float64
wtd_mean_Density	float64

gmean_Density	float64
wtd_gmean_Density	float64
entropy_Density	float64
wtd_entropy_Density	float64
range_Density	float64
wtd_range_Density	float64
std_Density	float64
wtd_std_Density	float64
mean_ElectronAffinity	float64
wtd_mean_ElectronAffinity	float64
gmean_ElectronAffinity	float64
wtd_gmean_ElectronAffinity	float64
entropy_ElectronAffinity	float64
wtd_entropy_ElectronAffinity	float64
range_ElectronAffinity	float64
wtd_range_ElectronAffinity	float64
std_ElectronAffinity	float64
wtd_std_ElectronAffinity	float64
mean_FusionHeat	float64
wtd_mean_FusionHeat	float64
gmean_FusionHeat	float64
wtd_gmean_FusionHeat	float64
entropy_FusionHeat	float64
wtd_entropy_FusionHeat	float64
range_FusionHeat	float64
wtd_range_FusionHeat	float64
std_FusionHeat	float64
wtd_std_FusionHeat	float64
mean_ThermalConductivity	float64
wtd_mean_ThermalConductivity	float64
gmean_ThermalConductivity	float64
wtd_gmean_ThermalConductivity	float64
entropy_ThermalConductivity	float64

2. Attributes in **unique_m.csv**: Chemical formula – Categorical type

Other attributes – Quantitative type

H	float64
He	int64
Li	float64
Be	float64
B	float64
C	float64
N	float64
O	float64
F	float64

Ne	int64
Na	float64
Mg	float64
Al	float64
Si	float64
P	float64
S	float64
Cl	float64
Ar	int64
K	float64
Ca	float64
Sc	float64
Ti	float64
V	float64
Cr	float64
Mn	float64
Fe	float64
Co	float64
Ni	float64
Cu	float64
Zn	float64
Ga	float64
Ge	float64
As	float64
Se	float64
Br	float64
Kr	int64
Rb	float64
Sr	float64
Y	float64
Zr	float64
Nb	float64
Mo	float64
Tc	float64
Ru	float64
Rh	float64
Pd	float64
Ag	float64
Cd	float64
In	float64
Sn	float64
Sb	float64
Te	float64
I	float64
Xe	int64
Cs	float64
Ba	float64
La	float64

Ce	float64
Pr	float64
Nd	float64
Pm	int64
Sm	float64
Eu	float64
Gd	float64
Tb	float64
Dy	float64
Ho	float64
Er	float64
Tm	float64
Yb	float64
Lu	float64
Hf	float64
Ta	float64
W	float64
Re	float64
Os	float64
Ir	float64
Pt	float64
Au	float64
Hg	float64
Tl	float64
Pb	float64
Bi	float64
Po	int64
At	int64
Rn	int64
critical_temp	float64
material	object

Hence, we see that the attributes in train.csv are all quantitative and the attributes in unique_m.csv are also quantitative except the material attribute, which is categorical.

■ TASK ABSTRACTION

QUESTIONS EXPLORED IN OUR DATASET:

1. How do the different attributes vary with critical temperature?
2. Can we quantify the contribution of each attribute (physical/chemical properties) towards the trend in target (critical temperature) in train.csv?
3. What metrics of the attributes show the strongest correlations on critical temperature?
4. What are the most significant metrics from each attribute class that affect the behaviour of each material's critical temperature?

5. From the previously claimed correlation results, how can we visualize the strength and nature of dependency of each of the selected metrics on critical temperature?
6. Given the industry's requirement of temperature ranges, what type of elements will be available for them to construct a superconducting material, and in what quantities?
7. For a feasible temperature range and a specific elemental series, can we predict the composition of the superconductor?
8. How many superconductors have a certain element, such as copper, iron or zinc, as their constituent?

INVESTIGATION CARRIED OUT TO ANSWER THE POSED QUESTIONS:

1. **Attribute:** Some randomly chosen attributes to see the initial variations of the data. [train.csv]

We plot the different attributes against critical temperature in the independent axis, to see the general trends readily available from the dataset. This helps us further decide on which type of visualization techniques are to be employed in order to carry out further investigations.

2. **Attribute:** Critical temperature – target attribute; All the attributes are tested for dependence on the target variables. [train.csv]

We attempt to quantify the contribution of each attribute to the trend in the target. We plot a correlation matrix using Kendall's rank correlation coefficient method, which is a statistical method to measure the degree of ordinal association between two measured quantities. Thus, we obtain the strength of dependence of each property on critical temperature.

3. **Attribute:** All the attributes [train.csv]

We sort the correlation coefficients obtained corresponding to the critical temperature column from the previously obtained matrix. We visualize this using a heatmap with the annotations being the corresponding correlation coefficients.

4. **Attribute:** All the attributes except critical_temp (critical temperature) [train.csv]

Using a scatter plot, we plot the absolute values of the correlation coefficients, colour-coding the sign of the values by red (negative) and blue (positive). Using this visualization, we obtain the most significant metrics that are affecting the trend in critical temperature. Now, we consider each attribute class, and find the most significant metric out of that class.

5. **Attributes:** number_of_elements, wtd_entropy_atomic_mass, range_fie, range_atomic_radius, gmean_Density, entropy_ElectronAffinity, entropy_FusionHeat, range_ThermalConductivity, wtd_gmean_Valence, critical_temp. [train.csv]

We observe the behaviour of each of these attributes and how the data is distributed, by plotting it against critical temperature.

6. Attribute: All the attributes except material. [unique_m.csv]

We divided the critical temperature into 5 quantiles, denoting temperature ranges. Now, we quantify the stoichiometric ratios of the elements in each series used for superconductors in each temperature range.

7. Attribute: critical_temp, alkali_metals, alkaline_earth_metals, transition_metals, posttransition_metals, lanthanoid_metals, metalloids, reactive_nonmetals, noble_gases. [Encoded attributes, derived from unique_m.csv]

We choose a temperature range and a specific elemental series. Now we plot the stoichiometric coefficients of each element used in the superconductors and visualize the density distribution. The densities of each element denote how much quantity we will require to construct the superconductor.

8. Attributes: contains_iron, contains_copper [Encoded attributes, derived from unique_m.csv]

A certain industry may be inclined for/against the usage of a certain element in their processes. Thus, it is important to be able to determine what fraction of the available superconductors contain those elements.

■ ENCODING

1. Since there is no categorical data in the dataset, for the sake of visualization we have used binning to analyze the data distribution by forming bins of continuous intervals across a specified number of quantiles. We associate the formed bins to the corresponding data and group the data to better analyze the behaviour.

The critical temperature of a superconductor is considerably important from the point of view of implementation. Different types of applications will have different requirements of ranges of temperatures for their purpose. Thus, we have binned the critical temperatures across pentiles and visualized the trend for each.

2. Since the element series in the periodic table plays a vital role, it has a considerable impact in the selection of a superconducting material. This is because the constituent elements' properties and availability are determined in a large way by these series, and this will play a large role when an industry is selecting a material for its implementation.

We implement an **extended version of label encoding** for numerically representing the labels that we created by classifying the elements into their corresponding elemental series, namely alkali metals, alkaline earth metals, transition metals, post-transition metals, lanthanides, metalloids, reactive non-metals and noble gases. To

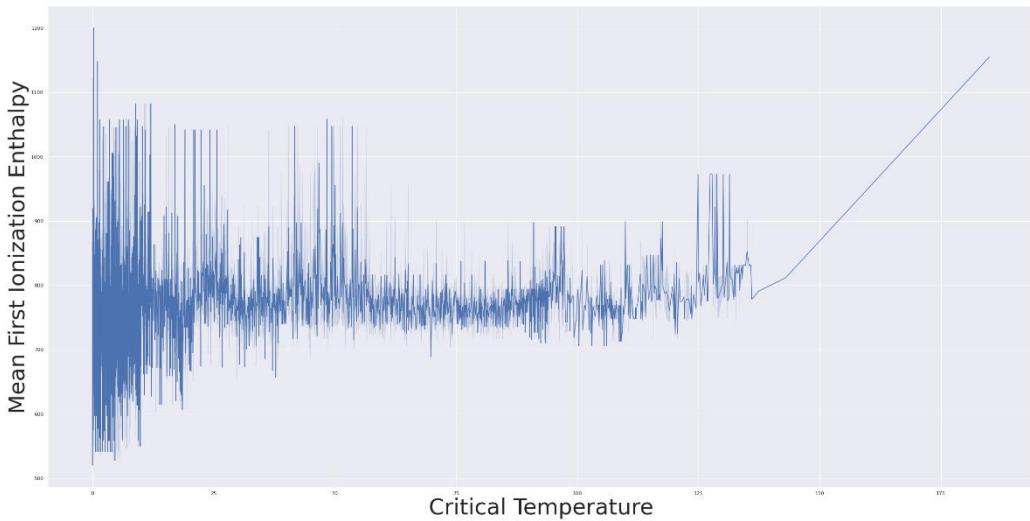
represent them in a numerical fashion, we select a corresponding value for each label, as the sum of the stoichiometric values of the constituent elements in the material.

Most of the encoding techniques are applied on categorical data, to convert them into a suitable form for analysis. However, almost all of the data in our dataset is of numerical type, and we require these numerical values itself for our visualization.

■ PLOTS:

Variation of the mean of attributes versus critical temperature: Initial exploration of data to observe any trends that we can use for further investigation

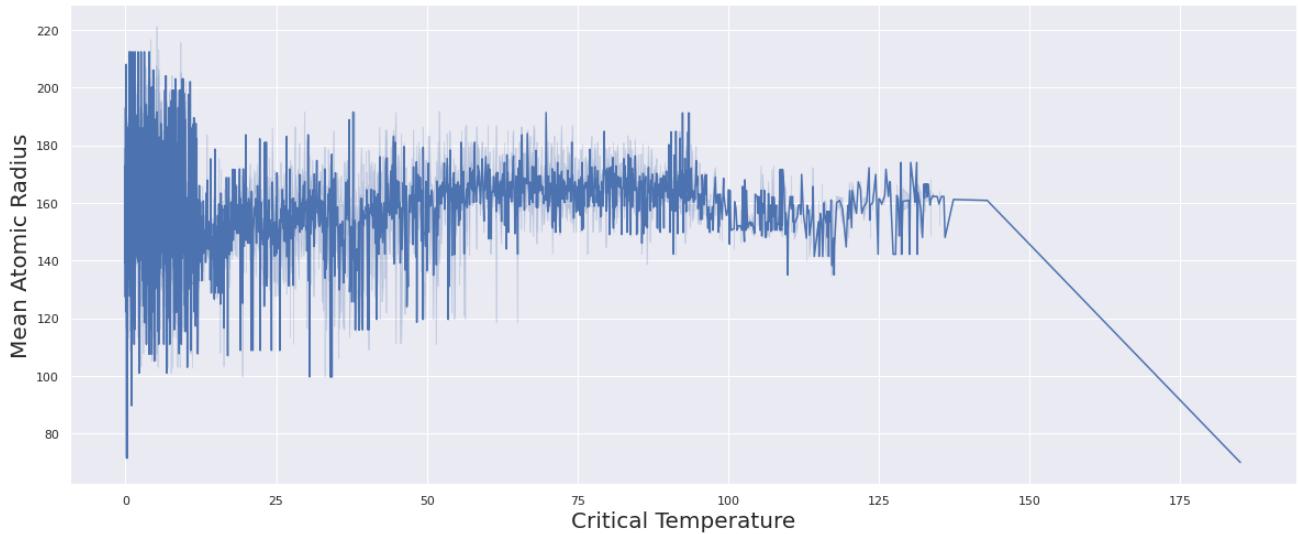
```
sns.set(rc={'figure.figsize':(40,20)})  
  
critical = sns.lineplot(x="critical_temp", y="mean_fie", data=attributes)  
  
critical.set_xlabel("Critical Temperature", fontsize = 50)  
  
critical.set_ylabel("Mean First Ionization Enthalpy", fontsize = 50)  
  
plt.show()
```



Lower ionization enthalpies at lower temperatures, rises steadily above 130 K

```
sns.set(rc={'figure.figsize':(40,20)})  
  
critical = sns.lineplot(x="critical_temp", y="mean_atomic_radius", data=attributes)  
  
critical.set_xlabel("Critical Temperature", fontsize = 50)  
  
critical.set_ylabel("Mean Atomic Radius", fontsize = 50)
```

```
plt.show()
```



Larger atoms constitute superconductors that operate at lower temperatures only. As the temperatures rise above 130K, the atomic size steadily drops.

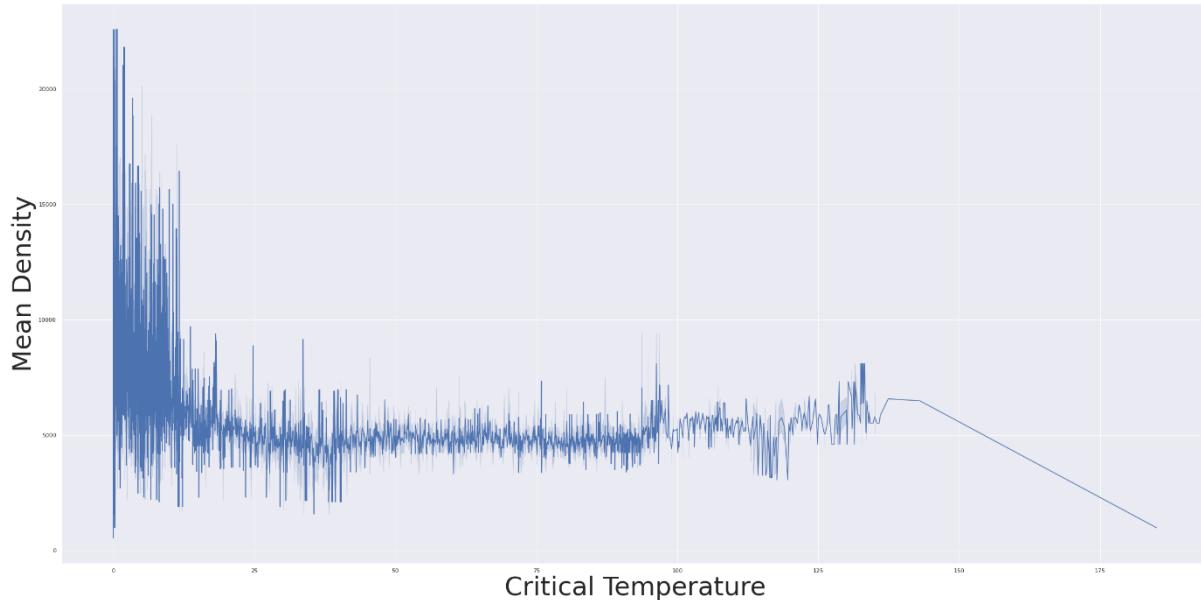
```
sns.set(rc={'figure.figsize':(40,20)})
```

```
critical = sns.lineplot(x="critical_temp", y="mean_Density", data=attributes)
```

```
critical.set_xlabel("Critical Temperature", fontsize = 50)
```

```
critical.set_ylabel("Mean Density", fontsize = 50)
```

```
plt.show()
```



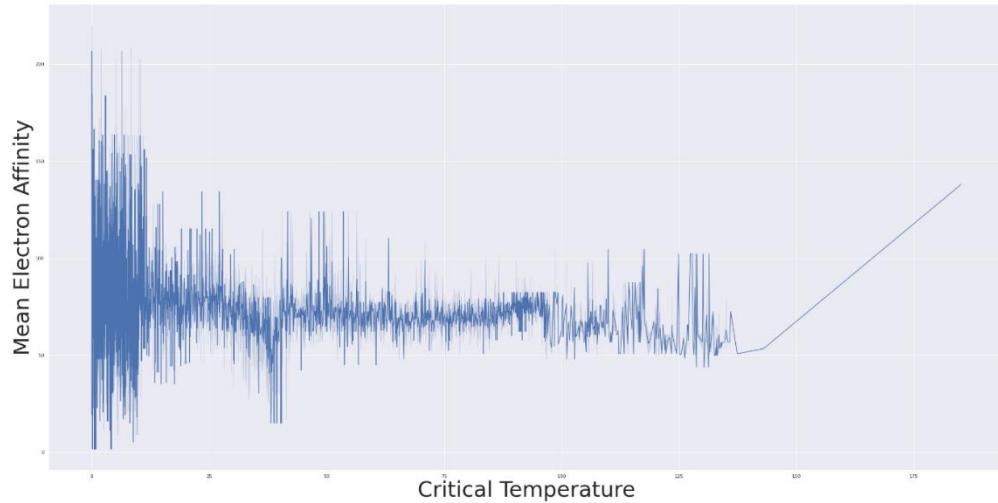
Denser superconductors exist at lower critical temperatures

```
sns.set(rc={'figure.figsize':(40,20)})
```

```

critical = sns.lineplot(x="critical_temp", y="mean_ElectronAffinity", data=attributes)
critical.set_xlabel("Critical Temperature", fontsize = 50)
critical.set_ylabel("Mean Electron Affinity", fontsize = 50)
plt.show()

```

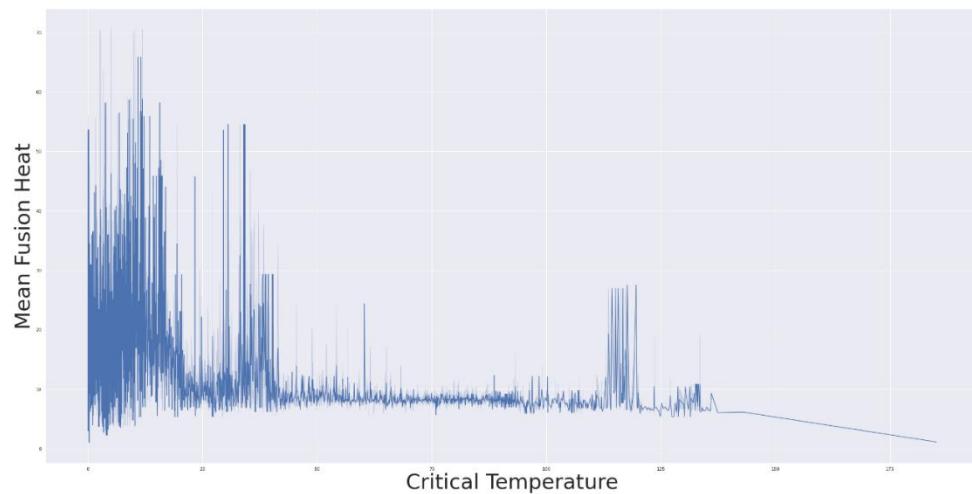


Electron affinity rises with rise in critical temperature. Non-metallic character, therefore, is visible in superconductors with high critical temperatures.

```

sns.set(rc={'figure.figsize':(40,20)})
critical = sns.lineplot(x="critical_temp", y="mean_FusionHeat", data=attributes)
critical.set_xlabel("Critical Temperature", fontsize = 50)
critical.set_ylabel("Mean Fusion Heat", fontsize = 50)
plt.show()

```



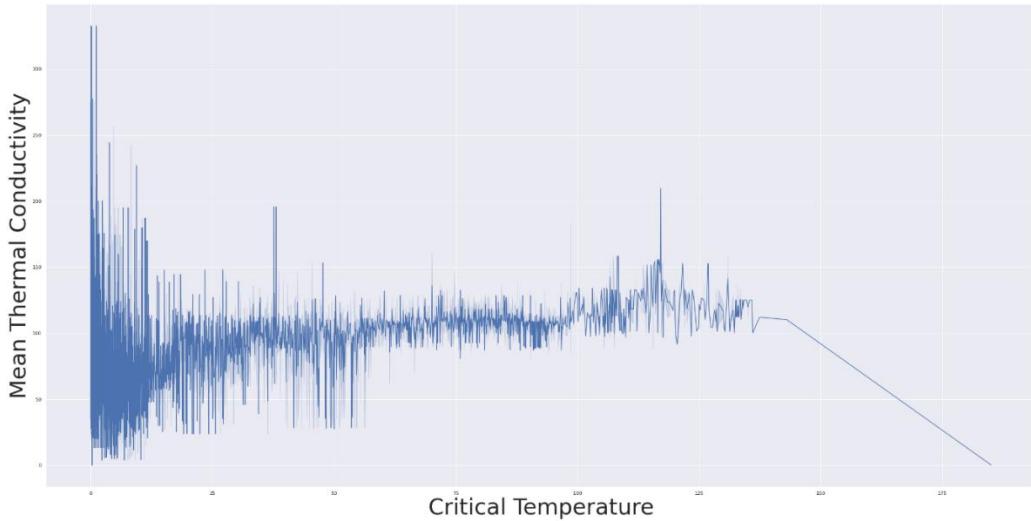
At higher temperatures, superconductors readily change states on addition of heat.

```
sns.set(rc={'figure.figsize':(40,20)})
```

```

critical = sns.lineplot(x="critical_temp", y="mean_ThermalConductivity", data=attributes)
critical.set_xlabel("Critical Temperature", fontsize = 50)
critical.set_ylabel("Mean Thermal Conductivity", fontsize = 50)
plt.show()

```

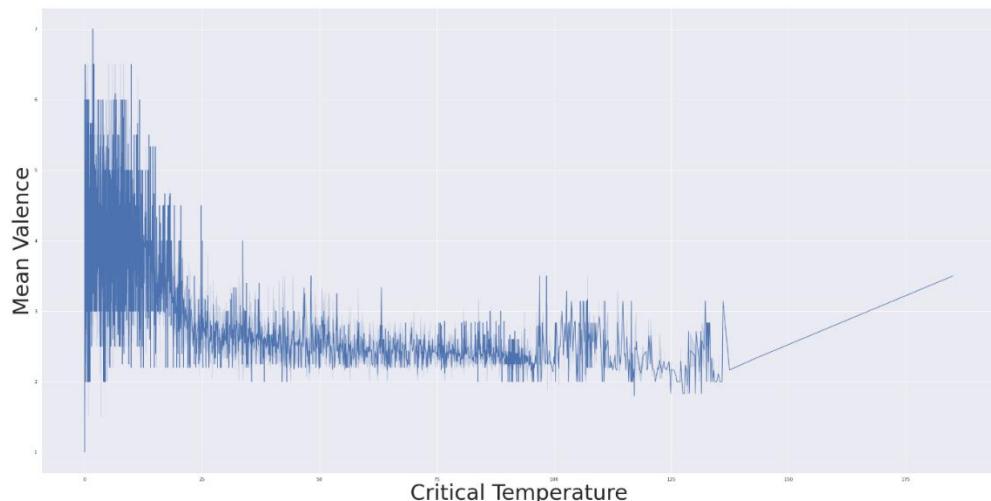


Thermal conductivity decreases with rise in critical temperature. This is consistent with the trends in electron affinity and first ionization enthalpy

```

sns.set(rc={'figure.figsize':(40,20)})
critical = sns.lineplot(x="critical_temp", y="mean_Valence", data=attributes)
critical.set_xlabel("Critical Temperature", fontsize = 50)
critical.set_ylabel("Mean Valence", fontsize = 50)
plt.show()

```



Valence decreases slightly, before increasing again.

Conclusion: At extremely low critical temperatures, a lot of different superconductors exists, around 0K. As the temperature rises, the properties gradually become more specific and start to show distinct trends.

Segregating the superconducting materials based on whether a particular element is present in it or not

```
mat_data['contains_iron']=pd.cut(mat_data['Fe'],bins=[-1,0.000001,10000],labels=['Non-iron','Iron'])

mat_data['contains_copper']=pd.cut(mat_data['Cu'],bins=[-1,0.000001,10000],labels=['Non-copper','Copper'])

fe_count=mat_data['contains_iron'].value_counts()

mat_content_dat_fe = pd.DataFrame(fe_count).reset_index()

mat_content_dat_fe.columns=['mat_content','count']

cu_count=mat_data['contains_copper'].value_counts()

mat_content_dat_cu= pd.DataFrame(cu_count).reset_index()

mat_content_dat_cu.columns=['mat_content','count']

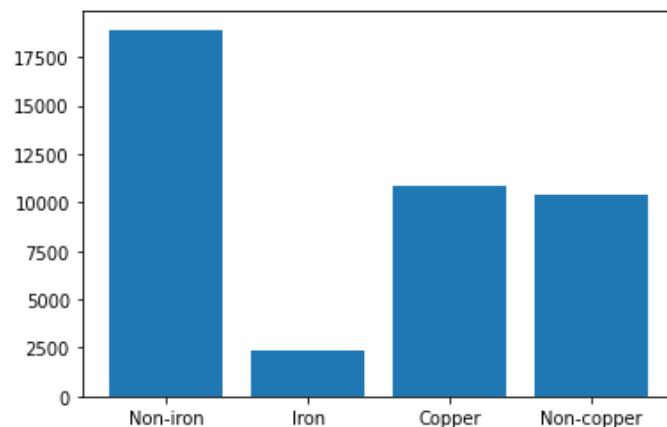
mat_content_dat_cu.index=[2,3]

frames=[mat_content_dat_fe,mat_content_dat_cu]

mat_content_dat=pd.concat(frames)

plt.bar(mat_content_dat['mat_content'],mat_content_dat['count'])

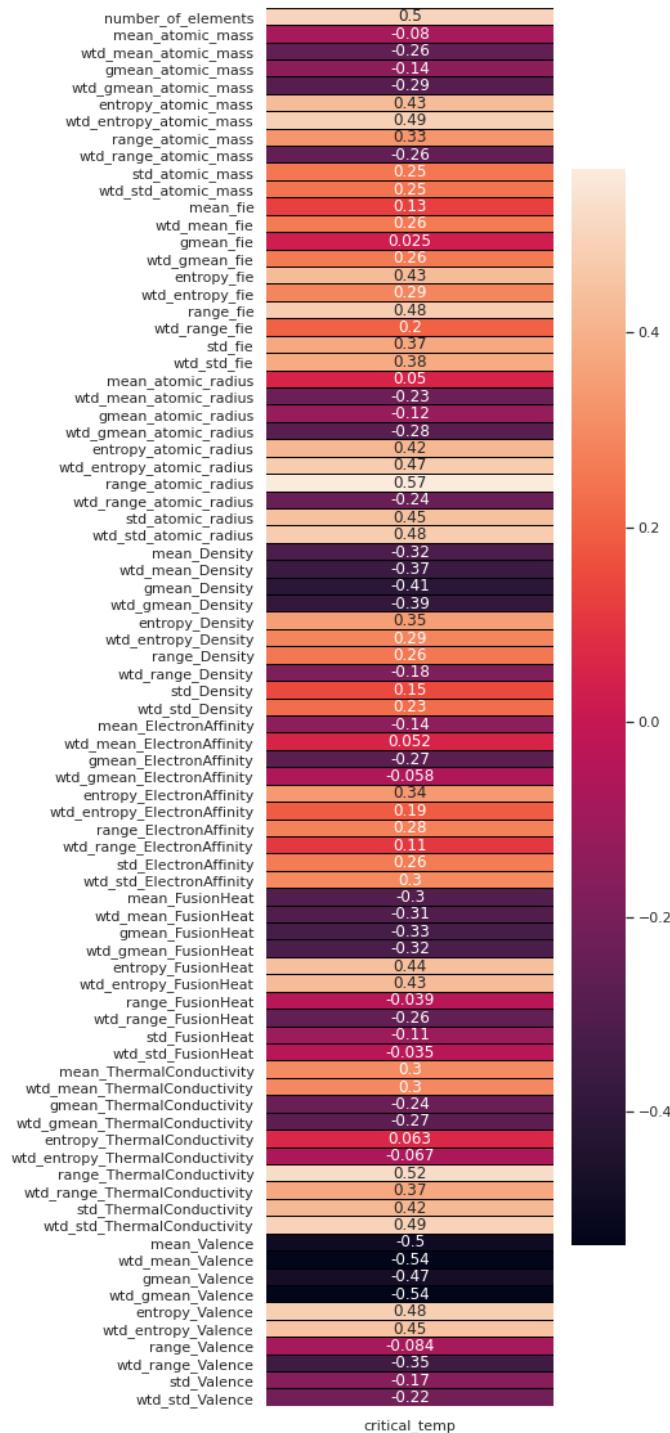
plt.show()
```



This bar-plot reports summary statistics on iron-based versus non-iron, and copper versus non-copper superconductor materials. The size is the total number of observations of the material out of 21,263 materials.

Study of dependency of the attributes with critical temperature

```
correlation_data=data.corr(method='kendall')  
sn.set(rc={'figure.figsize':(5,20)})  
sn.heatmap(corr_rank,linedwidths=0.005,annot=True,linecolor="black")
```

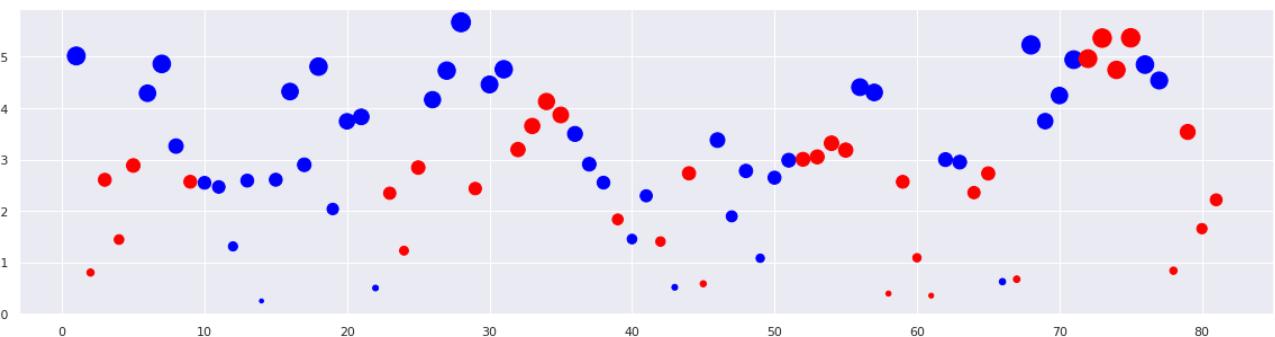


The heatmap shows the strength of dependence of each property on critical temperature with the annotations being the corresponding correlation coefficients. obtained via Kendall's rank correlation coefficient method

```

corr_df=pd.DataFrame(correlation_data['critical_temp'][0:-1]).reset_index()
corr_df.columns=['property','corr_factor']
corr_df['corr_sign']=pd.cut(corr_df['corr_factor'],bins=[-1,0,1],labels=["red","blue"])
corr_df['sl_no']=list(range(1,82))
corr_df['corr_factor']=corr_df['corr_factor'].abs()
plt.figure(figsize=(20,5))
plt.scatter(corr_df['sl_no'],corr_df['corr_factor'],c=corr_df['corr_sign'],s=corr_df['corr_factor']*500)
plt.show()

```

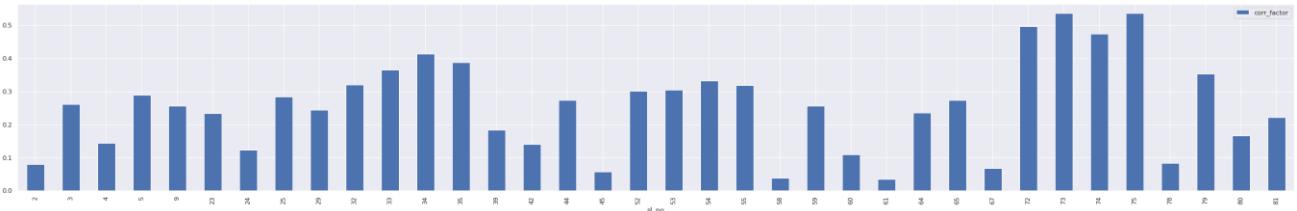


Scatter plot of correlation coefficients for all attributes with blue signifying positive correlation, red signifying negative correlation and size signifying strength of dependence

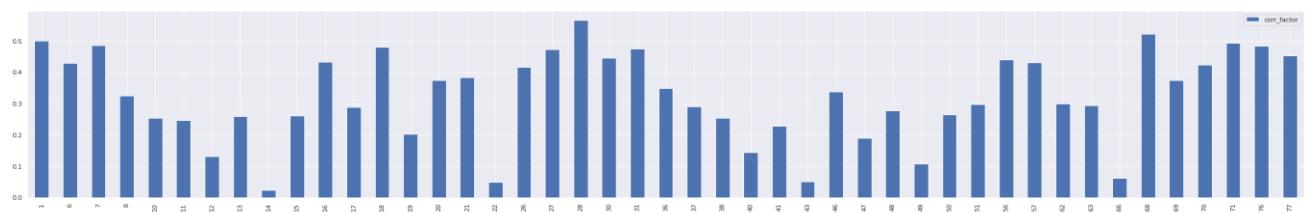
```

plt.figure(figsize=(20,5))
corr_df.groupby(['corr_sign']).plot(x="sl_no",y="corr_factor",kind="bar")

```



Bar plot of correlation coefficients for attributes showing negative correlation with critical temperature



Bar plot of correlation coefficients for attributes showing positive correlation with critical temperature

```
df_corr_ne=corr_df.iloc[[0]]
corr_atmass=corr_df.iloc[1:11]
corr_atmass=corr_atmass.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_am=corr_atmass.iloc[[9]]
corr_fie=corr_df.iloc[11:21]
corr_fie=corr_fie.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_fie=corr_fie.iloc[[9]]
corr_atrad=corr_df.iloc[21:31]
corr_atrad=corr_atrad.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_ar=corr_atrad.iloc[[9]]
corr_den=corr_df.iloc[31:41]
corr_den=corr_den.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_den=corr_den.iloc[[9]]
corr_eaff=corr_df.iloc[41:51]
corr_eaff=corr_eaff.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_ea=corr_eaff.iloc[[9]]
corr_fush=corr_df.iloc[51:61]
corr_fush=corr_fush.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_fh=corr_fush.iloc[[9]]
corr_thcon=corr_df.iloc[61:71]
corr_thcon=corr_thcon.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_tc=corr_thcon.iloc[[9]]
corr_val=corr_df.iloc[71:81]
corr_val=corr_val.sort_values(by=['corr_factor'],ignore_index=True)
df_corr_val=corr_val.iloc[[9]]
corr_frames=[df_corr_ne,df_corr_am,df_corr_fie,df_corr_ar,df_corr_den,df_corr_ea,df_corr_fh,df_corr_tc,df_corr_val]
df_corr=pd.concat(corr_frames).reset_index()
del(df_corr['index'])
df_corr
```

	property	corr_factor	corr_sign	sl_no
0	number_of_elements	0.501691	blue	1
1	wtd_entropy_atomic_mass	0.486195	blue	7
2	range_fie	0.480924	blue	18
3	range_atomic_radius	0.567212	blue	28
4	gmean_Density	0.413034	red	34
5	entropy_ElectronAffinity	0.337925	blue	46
6	entropy_FusionHeat	0.440881	blue	56
7	range_ThermalConductivity	0.523120	blue	68
8	wtd_gmean_Valence	0.536930	red	75

The most significant metrics from each attribute class that are affecting the trend in critical temperature

Visualizing the above metrics and re-establishing the results obtained

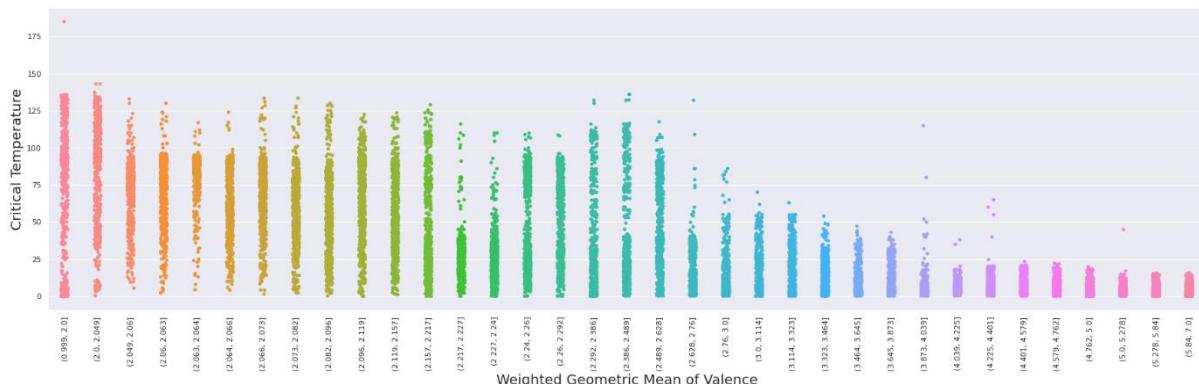
```
attributes['a'] = pd.qcut(attributes['wtd_gmean_Valence'], q=35, precision = 0)
print(attributes['a'].value_counts())
sns.set(rc={'figure.figsize':(30,8)})
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
critical.set_xlabel("Weighted Geometric Mean of Valence", fontsize = 20)
critical.set_ylabel("Critical Temperature", fontsize = 20)
plt.xticks(rotation=90)
plt.show()
del(attributes['a'])
```

(2.06, 2.063]	784
(2.76, 3.0]	762
(4.762, 5.0]	716
(0.999, 2.0]	692
(3.323, 3.464]	667
(2.24, 2.26]	649
(3.645, 3.873]	645
(2.157, 2.217]	640
(2.096, 2.119]	635
(2.066, 2.073]	630

```

(4.401, 4.579]      630
(5.278, 5.84]        628
(2.082, 2.096]       625
(4.225, 4.401]       614
(2.292, 2.386]       610
(2.064, 2.066]       608
(2.049, 2.06]        608
(2.489, 2.628]       608
(2.227, 2.24]        607
(3.114, 3.323]       607
(2.628, 2.76]        607
(2.386, 2.489]       605
(4.579, 4.762]       596
(3.873, 4.039]       592
(4.039, 4.225]       585
(2.073, 2.082]       584
(5.84, 7.0]           582
(2.217, 2.227]       575
(2.26, 2.292]        566
(2.119, 2.157]       563
(3.464, 3.645]       549
(2.0, 2.049]          523
(5.0, 5.278]          486
(3.0, 3.114]          454
(2.063, 2.064]        431
Name: a, dtype: int64

```



Weighted geometric mean of valence shows an almost linear decrease, consistent with the negative correlation coefficient obtained.

```

attributes['a'] = pd.qcut(attributes['range_ThermalConductivity'], q=4, precision = 0)
print(attributes['a'].value_counts())
sns.set(rc={'figure.figsize':(30,6)})
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
critical.set_xlabel("Range of Thermal Conductivity", fontsize = 20)
critical.set_ylabel("Critical Temperature", fontsize = 20)
# plt.xticks(rotation=90)

```

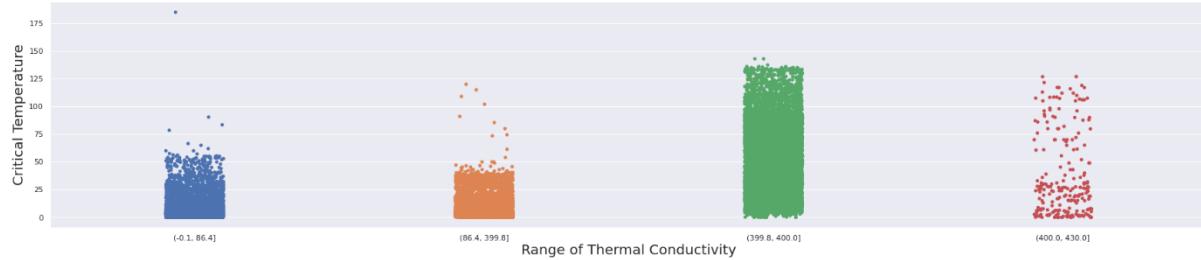
```

plt.show()

del(attributes['a'])

(399.8, 400.0]      10377
(86.4, 399.8]        5341
(-0.1, 86.4]         5316
(400.0, 430.0]        229
Name: a, dtype: int64

```



Thermal conductivity shows an almost linear increase, consistent with the positive correlation coefficient obtained. We also notice the high concentration of thermal conductivities in the (399.8, 400.0] quantile. We can conclude most superconducting materials possess thermal conductivities in this range.

```
attributes['a'] = pd.qcut(attributes['entropy_FusionHeat'], q=15, precision = 0)
```

```
print(attributes['a'].value_counts())
```

```
sns.set(rc={'figure.figsize':(30,6)})
```

```
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
```

```
critical.set_xlabel("Fusion Heat Entropy", fontsize = 20)
```

```
critical.set_ylabel("Critical Temperature", fontsize = 20)
```

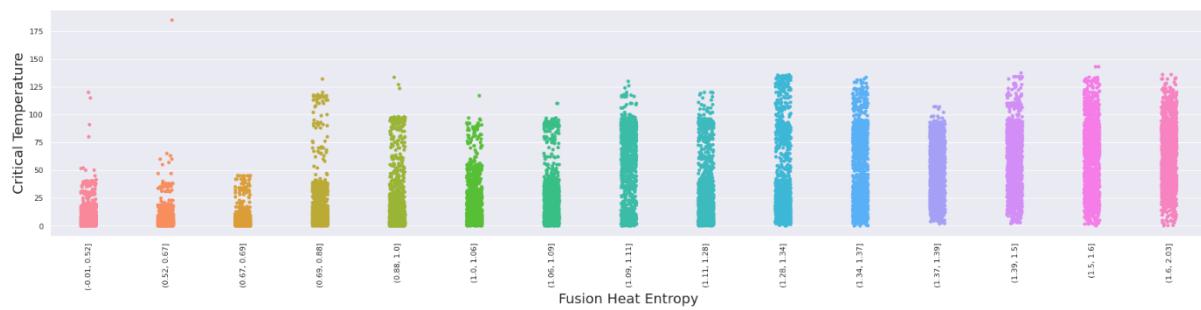
```
plt.xticks(rotation=90)
```

```
plt.show()
```

```
del(attributes['a'])
```

(1.28, 1.34]	1466
(0.88, 1.0]	1465
(1.39, 1.5]	1446
(-0.01, 0.52]	1435
(1.11, 1.28]	1427
(1.06, 1.09]	1427
(0.67, 0.69]	1424
(1.09, 1.11]	1417
(0.69, 0.88]	1412
(1.5, 1.6]	1402
(0.52, 0.67]	1400
(1.6, 2.03]	1396
(1.37, 1.39]	1393
(1.34, 1.37]	1384

```
(1.0, 1.06]      1369
Name: a, dtype: int64
```



Almost linear increase for fusion heat entropy, consistent with the positive correlation coefficient obtained for it.

```
attributes['a'] = pd.qcut(attributes['entropy_ElectronAffinity'], q=8, precision = 0)
```

```
print(attributes['a'].value_counts())
```

```
sns.set(rc={'figure.figsize':(30,6)})
```

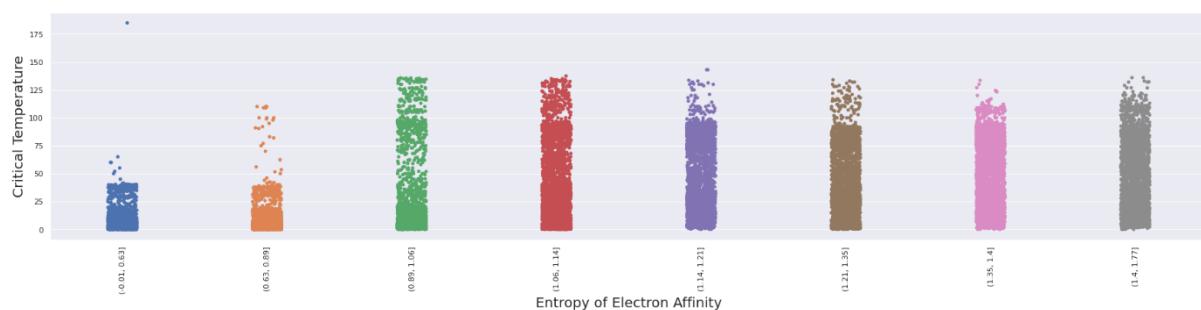
```
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
```

```
plt.xticks(rotation=90)
```

```
plt.show()
```

```
del(attributes['a'])
```

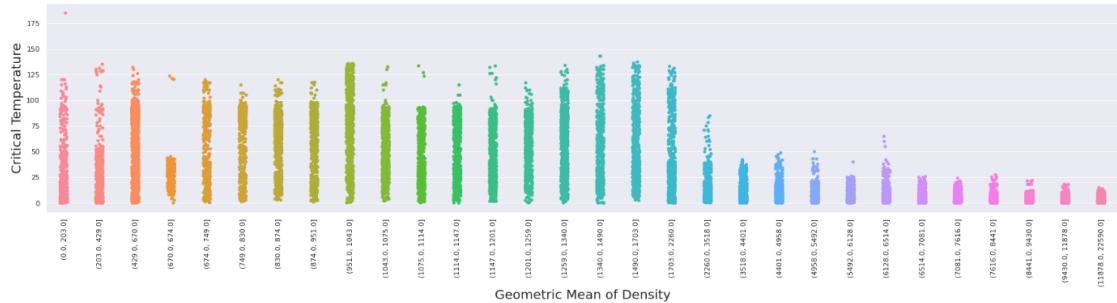
```
(1.35, 1.4]      2725
(1.06, 1.14]    2709
(-0.01, 0.63]   2664
(0.89, 1.06]    2659
(1.21, 1.35]    2654
(0.63, 0.89]    2652
(1.14, 1.21]    2613
(1.4, 1.77]     2587
Name: a, dtype: int64
```



Almost linear increase for entropy of electron affinity with critical temperature

```
attributes['a'] = pd.qcut(attributes['gmean_Density'], q=30, precision = 0)
print(attributes['a'].value_counts())
sns.set(rc={'figure.figsize':(30,6)})
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
critical.set_xlabel("Geometric Mean of Density", fontsize = 20)
critical.set_ylabel("Critical Temperature", fontsize = 20)
plt.xticks(rotation=90)
plt.show()
del(attributes['a'])

(429.0, 670.0]           1276
(1259.0, 1340.0]          818
(951.0, 1043.0]           808
(830.0, 874.0]             793
(1703.0, 2260.0]           744
(0.0, 203.0]                729
(9430.0, 11878.0]          725
(1114.0, 1147.0]            721
(203.0, 429.0]              720
(3518.0, 4401.0]             718
(6514.0, 7081.0]             713
(1201.0, 1259.0]             713
(6128.0, 6514.0]             712
(7081.0, 7616.0]             709
(8441.0, 9430.0]             708
(5492.0, 6128.0]             708
(4958.0, 5492.0]             706
(7616.0, 8441.0]             705
(4401.0, 4958.0]             697
(11878.0, 22590.0]            690
(1490.0, 1703.0]              680
(2260.0, 3518.0]              679
(749.0, 830.0]                 678
(1147.0, 1201.0]               675
(1075.0, 1114.0]               671
(1043.0, 1075.0]               664
(874.0, 951.0]                  627
(1340.0, 1490.0]                 623
(674.0, 749.0]                   492
(670.0, 674.0]                   361
Name: a, dtype: int64
```



Almost linear decrease, consistent with the negative correlation coefficient obtained.

```
attributes['a'] = pd.qcut(attributes['range_atomic_radius'], q=6, precision=0)
```

```
print(attributes['a'].value_counts())
```

```
sns.set(rc={'figure.figsize':(30,8)})
```

```
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
```

```
critical.set_xlabel("Range of Atomic Radius", fontsize = 20)
```

```
critical.set_ylabel("Critical Temperature", fontsize = 20)
```

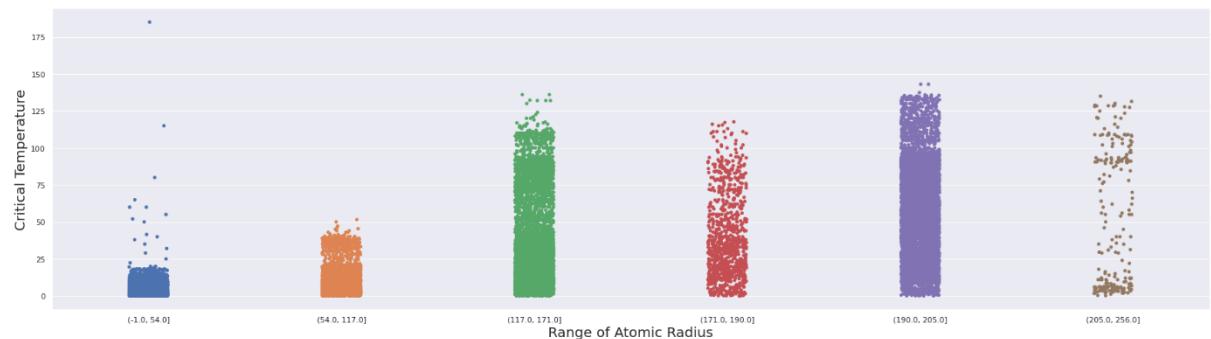
```
# plt.xticks(rotation=90)
```

```
plt.show()
```

```
del(attributes['a'])
```

(190.0, 205.0]	6729
(117.0, 171.0]	6266
(-1.0, 54.0]	3578
(54.0, 117.0]	3548
(171.0, 190.0]	917
(205.0, 256.0]	225

```
Name: a, dtype: int64
```



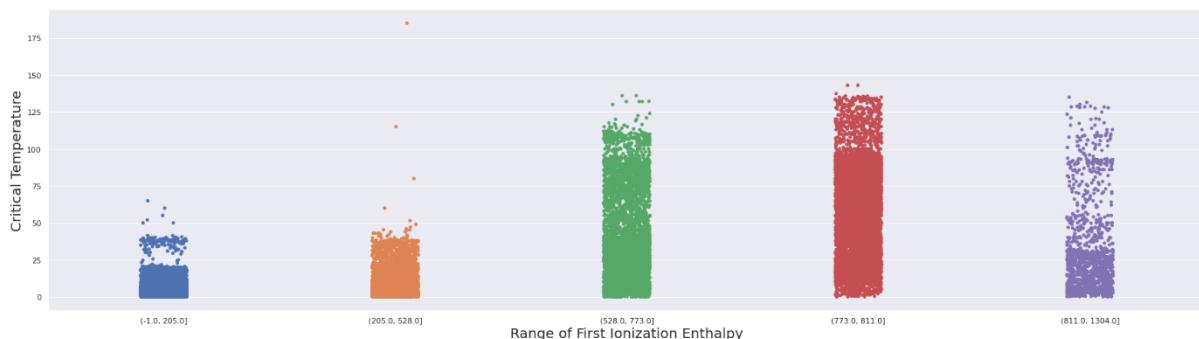
Almost linear increase, and most samples are concentrated in the 117-170 angstrom and 190 to 205 angstrom range.

```

attributes['a'] = pd.qcut(attributes['range_fie'], q=5, precision = 0)
print(attributes['a'].value_counts())
sns.set(rc={'figure.figsize':(30,8)})
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
critical.set_xlabel("Range of First Ionization Enthalpy", fontsize = 20)
critical.set_ylabel("Critical Temperature", fontsize = 20)
# plt.xticks(rotation=90)
plt.show()
del(attributes['a'])

(773.0, 811.0]      6784
(528.0, 773.0]      4586
(205.0, 528.0]      4314
(-1.0, 205.0]       4259
(811.0, 1304.0]     1320
Name: a, dtype: int64

```



Almost linear increase and most superconductors have first ionization enthalpies in the 528 kJ to 811 kJ, evident from the stripplot distribution

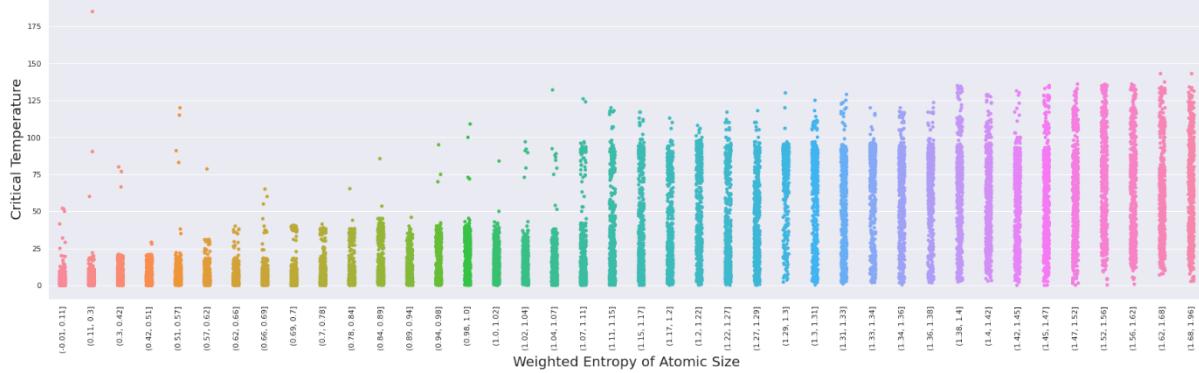
```

attributes['a'] = pd.qcut(attributes['wtd_entropy_atomic_mass'], q=40, precision = 0)
print(attributes['a'].value_counts())
sns.set(rc={'figure.figsize':(30,8)})
critical = sns.stripplot(x="a", y="critical_temp", data=attributes)
critical.set_xlabel("Weighted Entropy of Atomic Size", fontsize = 20)
critical.set_ylabel("Critical Temperature", fontsize = 20)
plt.xticks(rotation=90)
plt.show()
del(attributes['a'])

```

(1.07, 1.11]	568
(0.98, 1.0]	541
(1.36, 1.38]	536
(1.27, 1.29]	536
(0.51, 0.57]	534
(0.78, 0.84]	533
(1.33, 1.34]	533
(1.2, 1.22]	533
(0.62, 0.66]	533
(0.11, 0.3]	533
(0.89, 0.94]	532
(1.17, 1.2]	532
(0.94, 0.98]	532
(0.7, 0.78]	532
(1.02, 1.04]	532
(0.42, 0.51]	532
(1.62, 1.68]	532
(1.68, 1.96]	532
(-0.01, 0.11]	532
(1.4, 1.42]	532
(1.52, 1.56]	532
(1.45, 1.47]	532
(1.31, 1.33]	532
(1.42, 1.45]	531
(1.56, 1.62]	531
(1.47, 1.52]	531
(0.69, 0.7]	531
(1.15, 1.17]	531
(1.04, 1.07]	531
(0.84, 0.89]	530
(1.22, 1.27]	530
(1.34, 1.36]	530
(0.66, 0.69]	530
(0.3, 0.42]	530
(0.57, 0.62]	529
(1.3, 1.31]	529
(1.29, 1.3]	529
(1.38, 1.4]	527
(1.0, 1.02]	521
(1.11, 1.15]	496

Name: a, dtype: int64



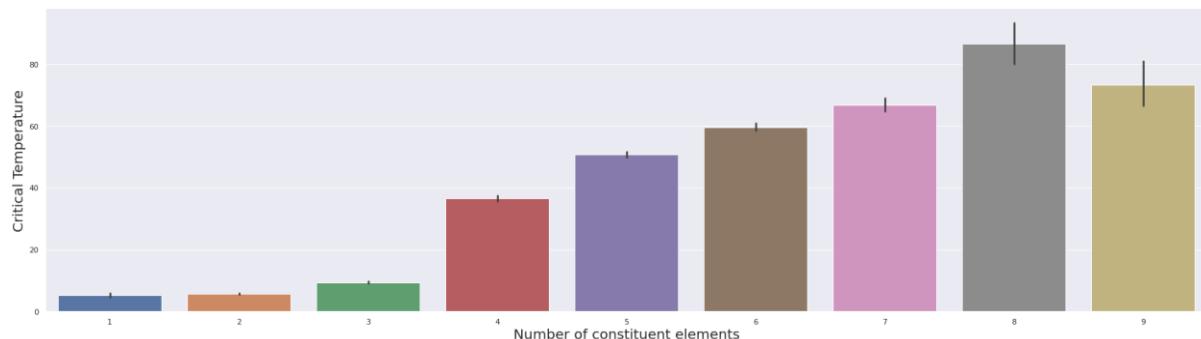
Almost linear increase of atomic size with increase in critical temperature, consistent with the positive correlation coefficient obtained.

```

attributes['a'] = pd.qcut(attributes['number_of_elements'], q=4, precision = 0)
print(attributes['a'].value_counts())
sns.set(rc={'figure.figsize':(30,8)})
critical = sns.barplot(x="number_of_elements", y="critical_temp", data=attributes)
critical.set_xlabel("Number of constituent elements", fontsize = 20)
critical.set_ylabel("Critical Temperature", fontsize = 20)
plt.show()
del(attributes['a'])

(0.0, 3.0]      7460
(4.0, 5.0]      5792
(3.0, 4.0]      4496
(5.0, 9.0]      3515
Name: a, dtype: int64

```



Almost linear increase of constituent elements with critical temperature, and most materials consist of 5 to 9 atoms

Analysis of materials used in superconductors:

Visualizing the presence of different elemental series in different critical temperature ranges

```

mat_df=mat_data

alkali_list=[list(mat_df.columns)[2],list(mat_df.columns)[10],list(mat_df.columns)[18],list(mat_df.columns)[36],list(mat_df.columns)[54]]

alkaline_list=[list(mat_df.columns)[3],list(mat_df.columns)[11],list(mat_df.columns)[19],list(mat_df.columns)[37],list(mat_df.columns)[55]]

transition_list=(list(mat_df.columns)[20:29])+(list(mat_df.columns)[38:47])+(list(mat_df.columns)[71:79])

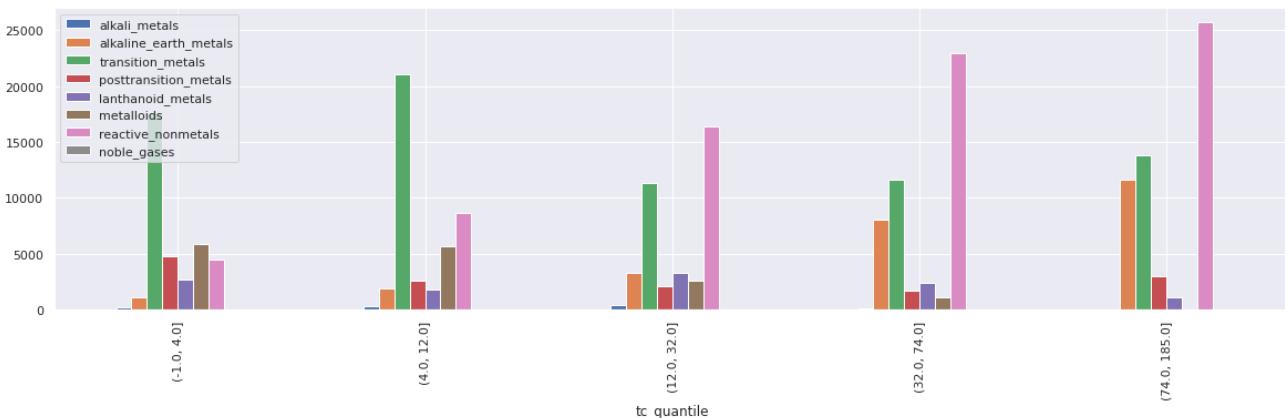
posttransition_list=list(mat_df.columns)[12:13]+list(mat_df.columns)[29:31]+list(mat_df.columns)[47:50]+list(mat_df.columns)[79:85]

```

```

lantha_list=list(mat_df.columns)[56:71]
metalloids_list=list(mat_df.columns)[4:5]+list(mat_df.columns)[13:14]+list(mat_df.columns)[31:33]+list(mat_df.columns)[50:52]
nonmetals_list=list(mat_df.columns)[0:1]+list(mat_df.columns)[5:9]+list(mat_df.columns)[14:17]+list(mat_df.columns)[33:35]+list(mat_df.columns)[52:53]
noble_list=[list(mat_df.columns)[1],list(mat_df.columns)[9],list(mat_df.columns)[17],list(mat_df.columns)[35],list(mat_df.columns)[53],list(mat_df.columns)[85]]
mat_df['alkali_metals']=mat_df[alkali_list].sum(axis=1)
mat_df['alkaline_earth_metals']=mat_df[alkaline_list].sum(axis=1)
mat_df['transition_metals']=mat_df[transition_list].sum(axis=1)
mat_df['posttransition_metals']=mat_df[posttransition_list].sum(axis=1)
mat_df['lanthanoid_metals']=mat_df[lantha_list].sum(axis=1)
mat_df['metalloids']=mat_df[metalloids_list].sum(axis=1)
mat_df['reactive_nonmetals']=mat_df[nonmetals_list].sum(axis=1)
mat_df['noble_gases']=mat_df[noble_list].sum(axis=1)
mat_df['tc_quantile']=pd.qcut(mat_df['critical_temp'],q=5,precision=0)
mat_class_df=mat_df.iloc[:,90:99]
mat_class_df.groupby(['tc_quantile']).sum().plot(kind='bar',figsize=(20,5))

```



Visualizing the presence of different elemental series in different critical temperature ranges

Visualizing the presence of elements in a particular elemental series by their stoichiometric coefficients in the superconducting materials

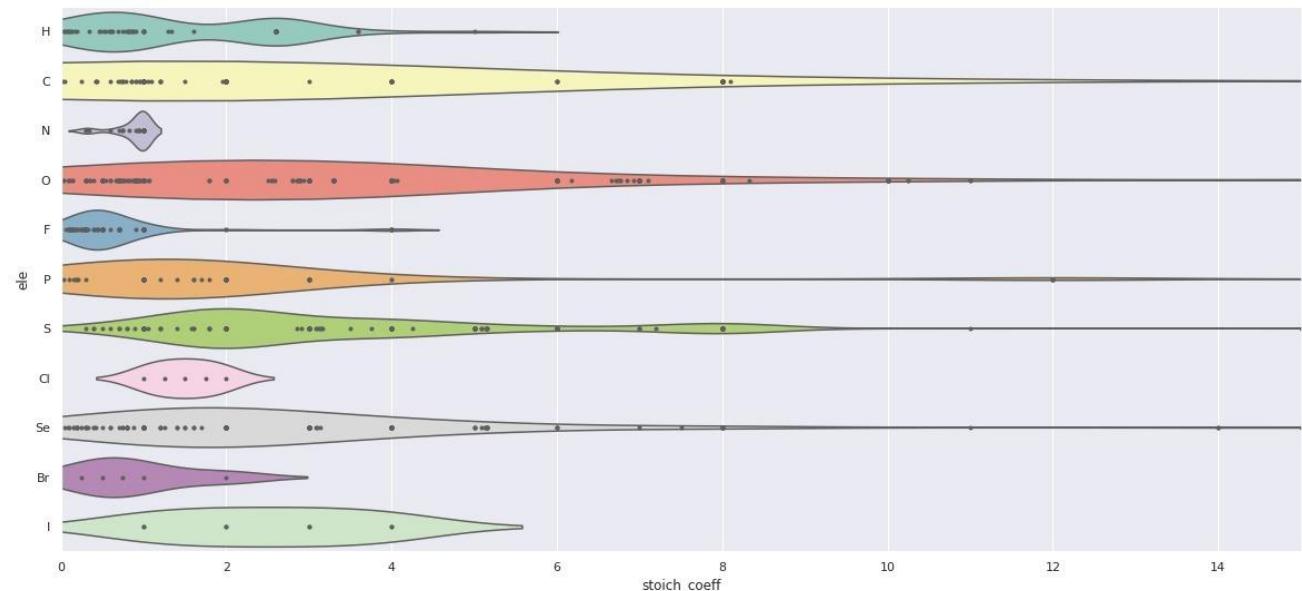
```
desirable_df=mat_df.loc[mat_df['tc_quantile']==mat_df['tc_quantile'].unique()[4]]
```

```
des_nonmetal=desirable_df[nonmetals_list]
des_H=pd.DataFrame(des_nonmetal['H'])
des_H.columns=['stoich_coeff']
des_H['ele']='H'
des_C=pd.DataFrame(des_nonmetal['C'])
des_C.columns=['stoich_coeff']
des_C['ele']='C'
des_N=pd.DataFrame(des_nonmetal['N'])
des_N.columns=['stoich_coeff']
des_N['ele']='N'
des_O=pd.DataFrame(des_nonmetal['O'])
des_O.columns=['stoich_coeff']
des_O['ele']='O'
des_F=pd.DataFrame(des_nonmetal['F'])
des_F.columns=['stoich_coeff']
des_F['ele']='F'
des_P=pd.DataFrame(des_nonmetal['P'])
des_P.columns=['stoich_coeff']
des_P['ele']='P'
des_S=pd.DataFrame(des_nonmetal['S'])
des_S.columns=['stoich_coeff']
des_S['ele']='S'
des_Cl=pd.DataFrame(des_nonmetal['Cl'])
des_Cl.columns=['stoich_coeff']
des_Cl['ele']='Cl'
des_Se=pd.DataFrame(des_nonmetal['Se'])
des_Se.columns=['stoich_coeff']
des_Se['ele']='Se'
des_Br=pd.DataFrame(des_nonmetal['Br'])
des_Br.columns=['stoich_coeff']
```

```

des_Br['ele']='Br'
des_I=pd.DataFrame(des_nonmetal['I'])
des_I.columns=['stoich_coeff']
des_I['ele']='I'
des_frames=[des_H,des_C,des_N,des_O,des_F,des_P,des_S,des_Cl,des_Se,des_Br,des_I]
des_nonmetal=pd.concat(des_frames).reset_index()
del(des_nonmetal['index'])
sn.set(rc={'figure.figsize':(20,9)})
plot_nonmetals=sn.violinplot(x="stoich_coeff",y="ele",data=des_nonmetal[des_nonmetal['stoich_coeff']>0],scale="width",palette="Set3",inner="points")
plot_nonmetals=plot_nonmetals.set(xlim=(0,12))

```



Visualizing the presence of elements in the non-metal series by their stoichiometric coefficients in the materials in the last critical temperature quantile (74 K - 185 K)

```

des_Cu=pd.DataFrame(des_transition['Cu'])
des_Cu.columns=['stoich_coeff']
des_Cu['ele']='Cu'
des_Y=pd.DataFrame(des_transition['Y'])
des_Y.columns=['stoich_coeff']
des_Y['ele']='Y'

```

```

des_Ni=pd.DataFrame(des_transition['Ni'])
des_Ni.columns=['stoich_coeff']
des_Ni['ele']='Ni'

des_Fe=pd.DataFrame(des_transition['Fe'])
des_Fe.columns=['stoich_coeff']
des_Fe['ele']='Fe'

des_V=pd.DataFrame(des_transition['V'])
des_V.columns=['stoich_coeff']
des_V['ele']='V'

des_Ag=pd.DataFrame(des_transition['Ag'])
des_Ag.columns=['stoich_coeff']
des_Ag['ele']='Ag'

des_tr_frames=[des_Cu,des_Y,des_Ni,des_Fe,des_V,des_Ag]

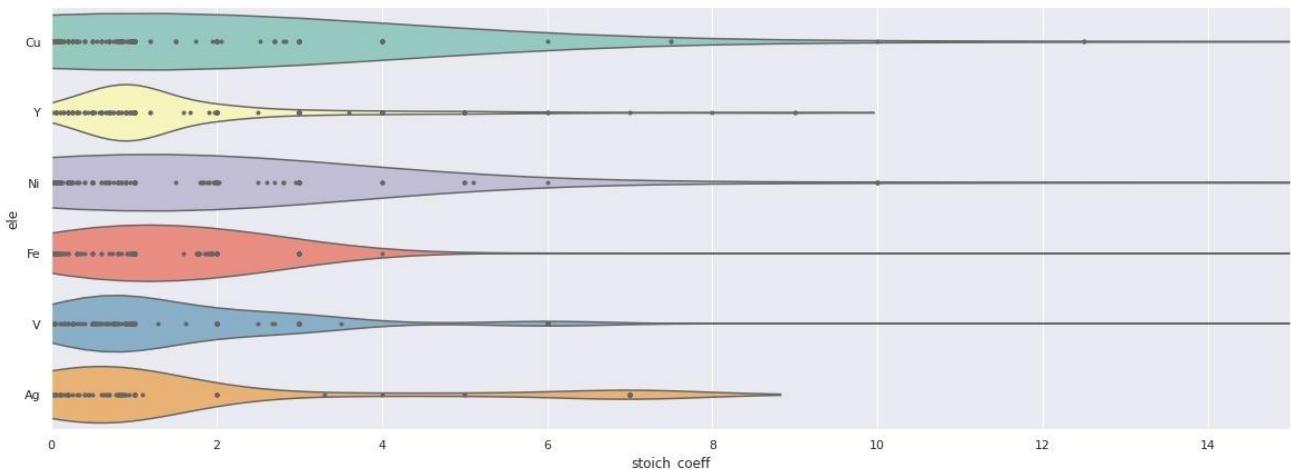
des_transition_metals=pd.concat(des_tr_frames).reset_index()

sn.set(rc={'figure.figsize':(20,7)})

plot_transition=sn.violinplot(x="stoich_coeff",y="ele",data=des_transition_metals[des_transition_metals['stoich_coeff']>0],scale="width",palette="Set3",inner="points")

plot_transition=plot_transition.set(xlim=(0,5))

```



Visualizing the presence of elements in the transition metal series by their stoichiometric coefficients in the last critical temperature quantile (74 K - 185 K)

```

des_alkaline=desirable_df[alkaline_list]
des_Be=pd.DataFrame(des_alkaline['Be'])

```

```

des_Be.columns=['stoich_coeff']
des_Be['ele']='Be'
des_Mg=pd.DataFrame(des_alkaline['Mg'])
des_Mg.columns=['stoich_coeff']
des_Mg['ele']='Mg'
des_Ca=pd.DataFrame(des_alkaline['Ca'])
des_Ca.columns=['stoich_coeff']
des_Ca['ele']='Ca'
des_Sr=pd.DataFrame(des_alkaline['Sr'])
des_Sr.columns=['stoich_coeff']
des_Sr['ele']='Sr'
des_Ba=pd.DataFrame(des_alkaline['Ba'])
des_Ba.columns=['stoich_coeff']
des_Ba['ele']='Ba'

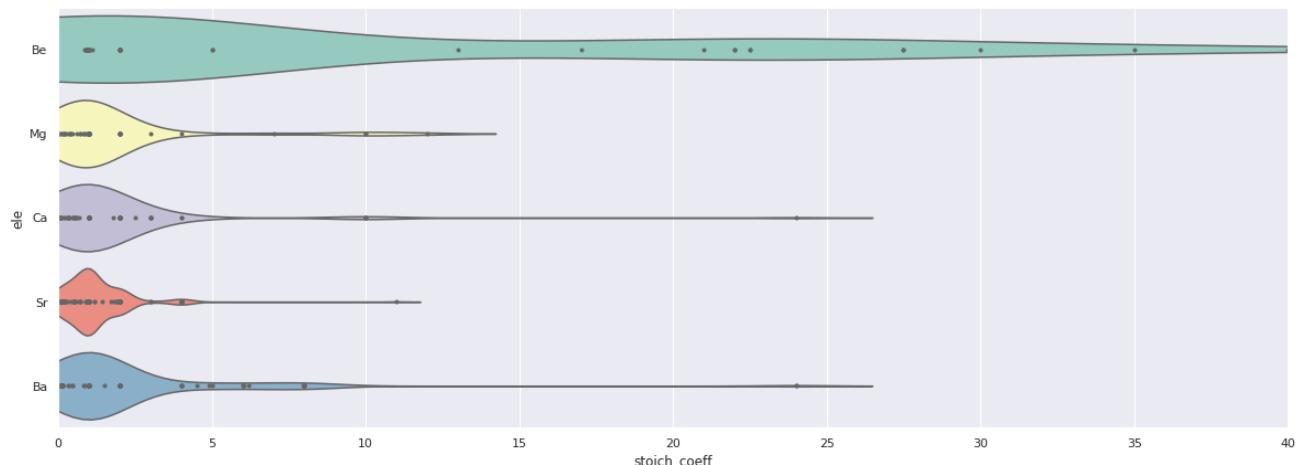
des_alkaline_frames=[des_Be,des_Mg,des_Ca,des_Sr,des_Ba]
des_alkaline=pd.concat(des_alkaline_frames).reset_index()
del(des_alkaline['index'])

sn.set(rc={'figure.figsize':(20,7)})

plot_alkaline=sn.violinplot(x="stoich_coeff",y="ele",data=des_alkaline[des_alkaline['stoich_coeff']>0],scale="width",palette="Set3",inner="points")

plot_alkaline=plot_alkaline.set(xlim=(0,4))

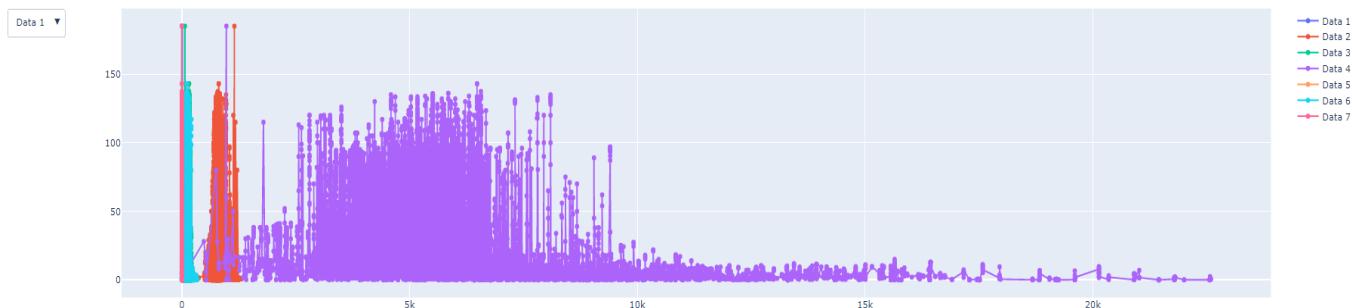
```



Visualizing the presence of elements in the alkaline earth metal series by their stoichiometric coefficients in a particular critical temperature range (74 K - 185 K)

REVIEW 2

PLOT 1: Preliminary investigation of properties

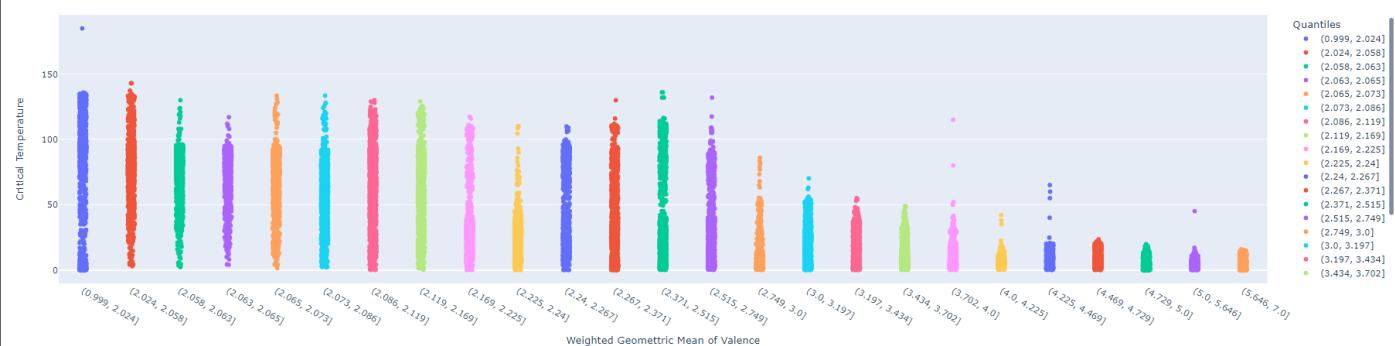


INFERENCES:

- Data 1: Lower ionization enthalpies at lower temperatures, rises steadily above 130 K
- Data 2: Larger atoms constitute superconductors that operate at lower temperatures only. As the temperatures rise above 130K, the atomic size steadily drops.
- Data 3: Denser superconductors exist at lower critical temperatures
- Data 4: Electron affinity rises with rise in critical temperature. Non-metallic character, therefore, is visible in superconductors with high critical temperatures.
- Data 5: At higher temperatures, superconductors readily change states on addition of heat.
- Data 6: Thermal conductivity decreases with rise in critical temperature. This is consistent with the trends in electron affinity and first ionization enthalpy
- Data 7: Valence decreases slightly, before increasing again.

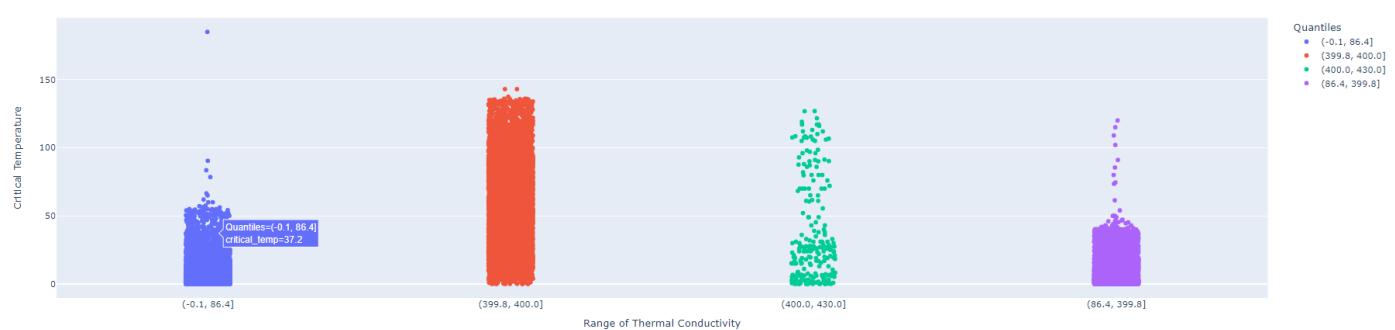
At extremely low critical temperatures, a lot of different superconductors exists, around 0K. As the temperature rises, the properties gradually become more specific and start to show distinct trends.

Weighted geometric mean of valence shows an almost linear decrease, consistent with the negative correlation coefficient obtained.



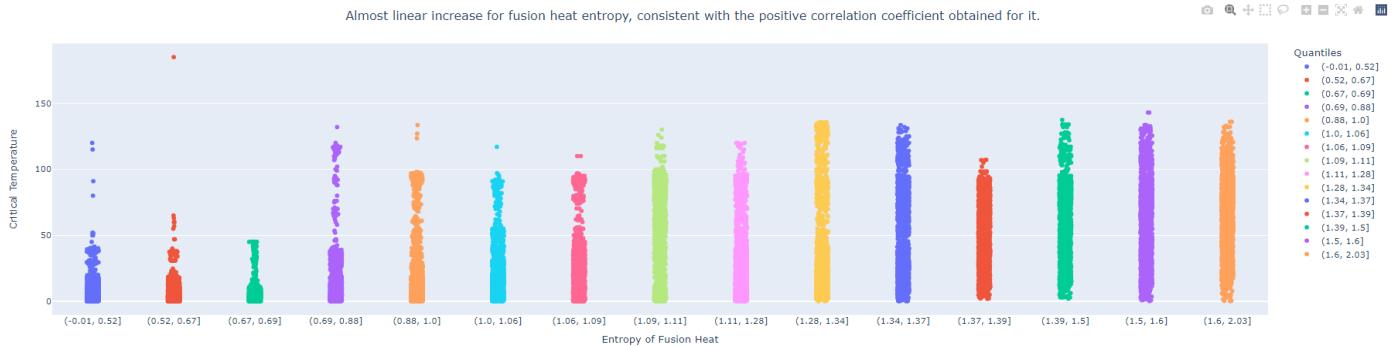
PLOT 2: Distribution of different quantiles of Range of Thermal Conductivity

Thermal conductivity shows an almost linear increase, consistent with the positive correlation coefficient obtained.



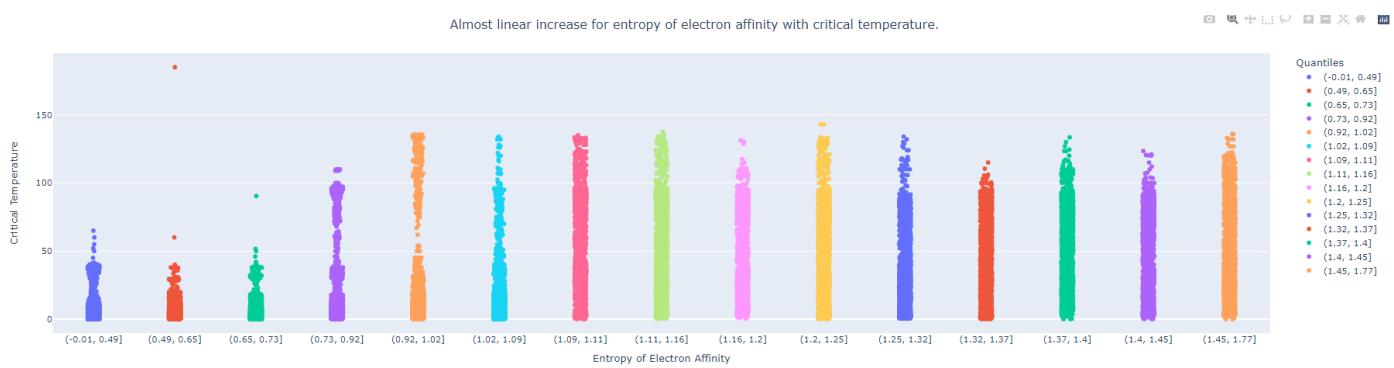
INFERRENCES: Thermal conductivity shows an almost linear increase, consistent with the positive correlation coefficient obtained. We also notice the high concentration of thermal conductivities in the (399.8 400.0] quantile. We can conclude most superconducting materials possess thermal conductivities in this range.

PLOT 3: Distribution of different quantiles of Entropy of Fusion Heat



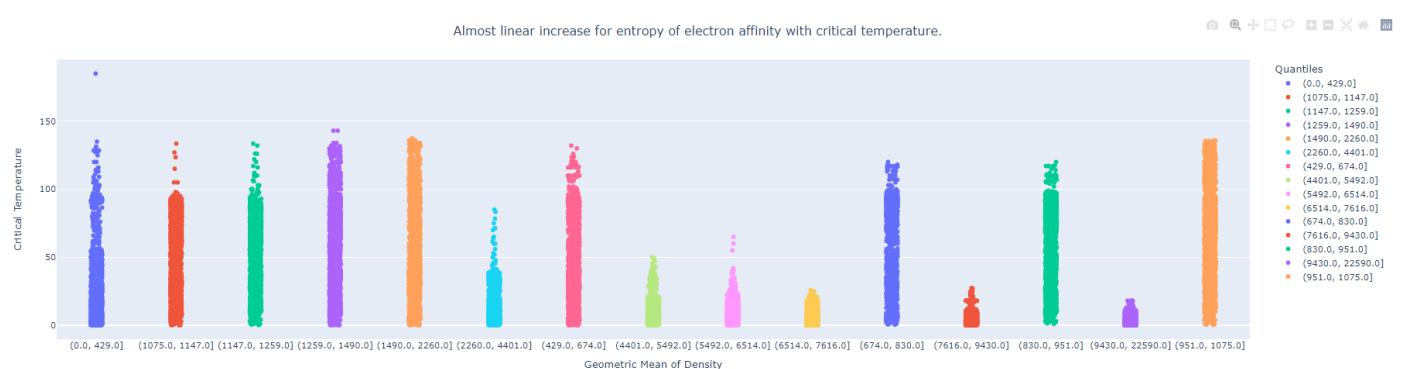
INFERRENCES: Almost linear increase for fusion heat entropy, consistent with the positive correlation coefficient obtained for it.

PLOT 4: Distribution of different quantiles of Entropy of Electron Affinity



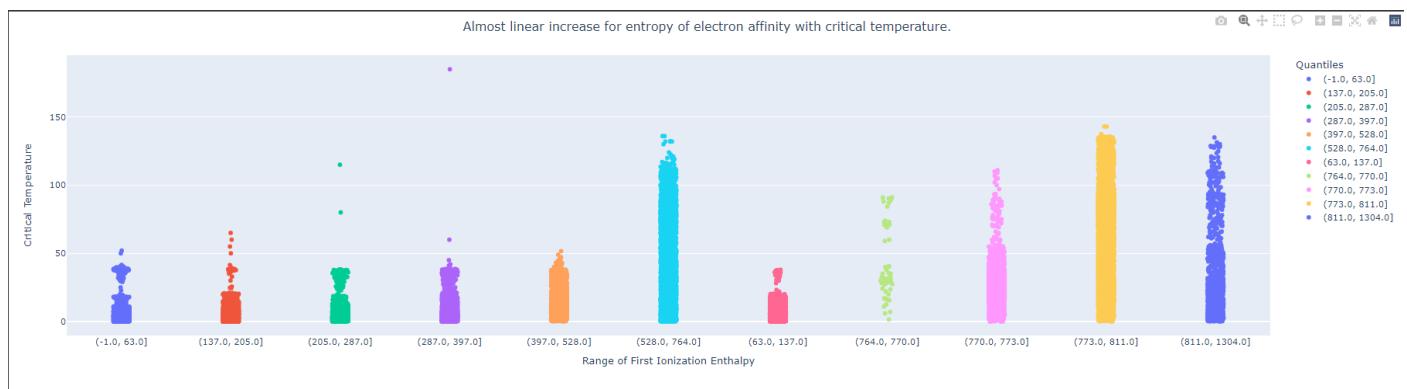
INFERRENCES: Almost linear increase for entropy of electron affinity with critical temperature.

PLOT 5: Distribution of different quantiles of Geometric Mean of Density



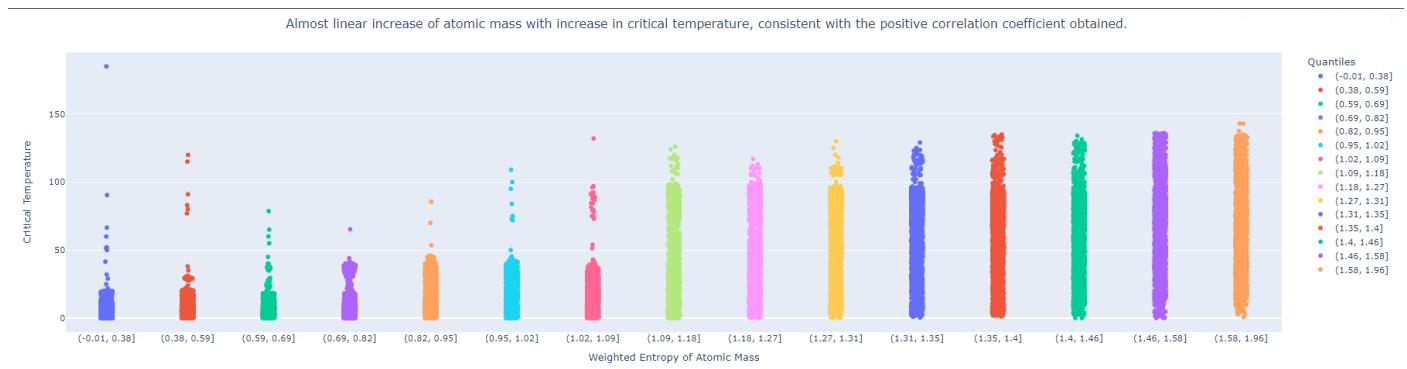
INFERRENCES: Almost linear decrease, consistent with the negative correlation coefficient obtained.

PLOT 6: Distribution of different quantiles of Range of First Ionization Enthalpy



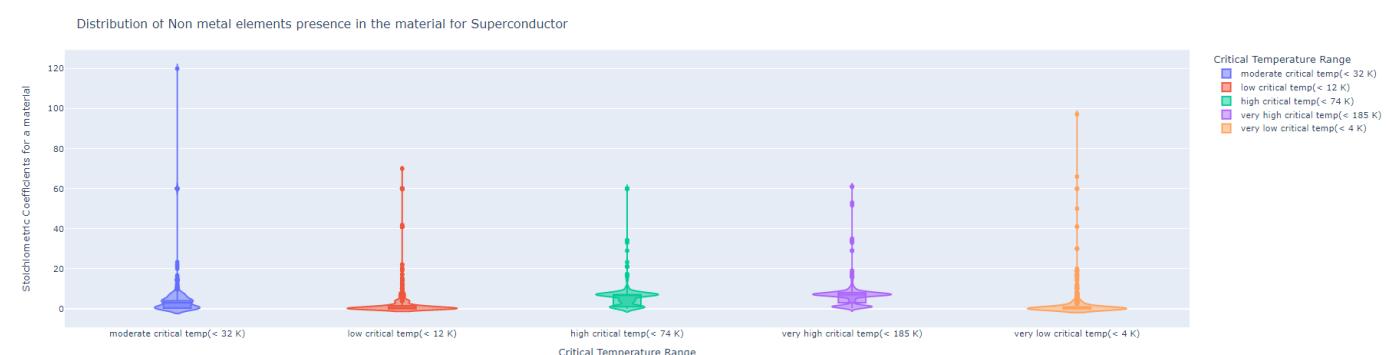
INFERENCES: Almost linear increase and most superconductors have first ionization enthalpies in the 528 kJ to 811 kJ, evident from the strip plot distribution.

PLOT 7: Distribution of different quantiles of Weighted Entropy of Atomic Mass



INFERENCES: Almost linear increase of atomic size with increase in critical temperature, consistent with the positive correlation coefficient obtained.

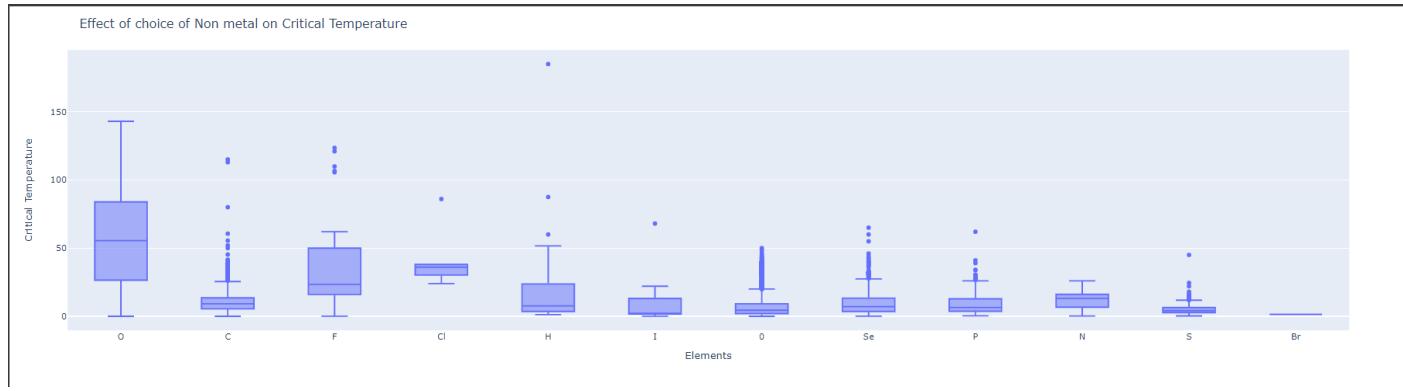
PLOT 8: Visualization to show how stoichiometric coefficients of each nonmetals present in a superconductor affect the critical temperature region in which the material behaves superconductor properties



INFERENCES: We see that there is a much larger presence of non-metals with the critical temperature 0 – 12 K that is, low and very low critical temperatures. Also, we see that in very low

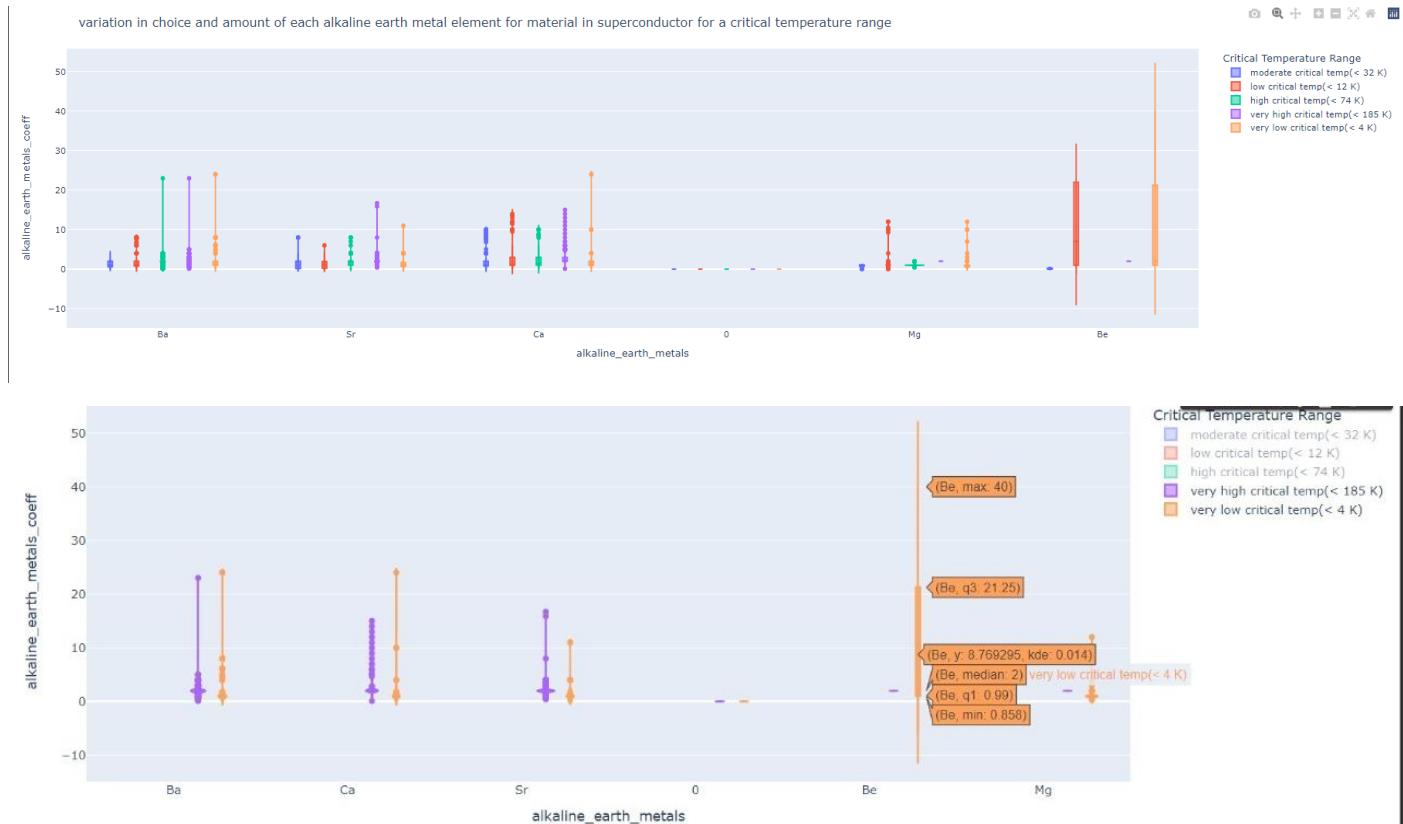
and moderate critical temperatures, there also tends to be high variability in the number of constituent elements in the superconductor.

PLOT 9: Visualization to observe distribution of critical temperature for materials containing a particular nonmetal

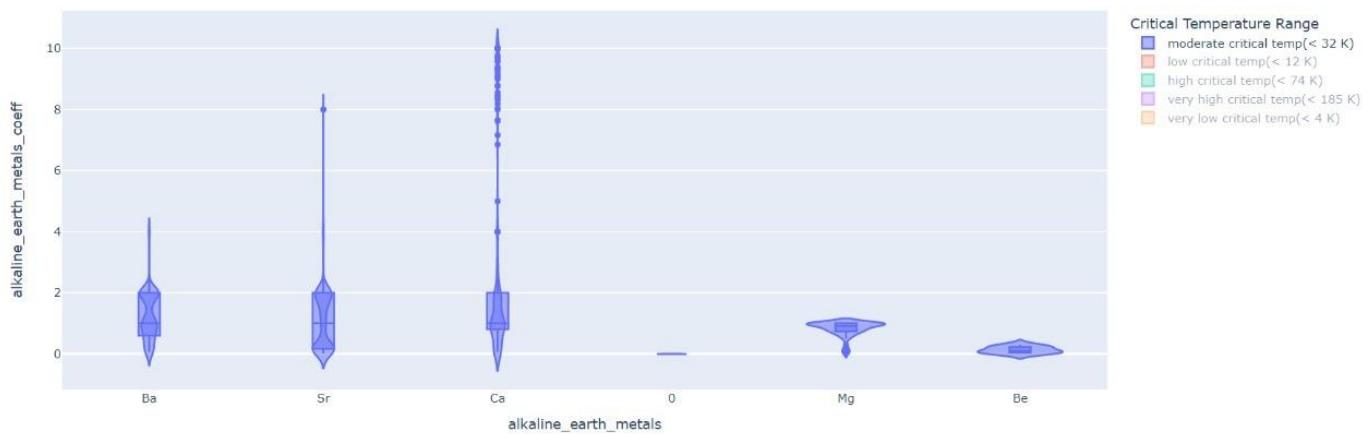


INFERENCES: We see those superconducting materials containing Oxygen (median temp: 55.45 K) exhibit higher critical temperatures than those containing Carbon (median temp: 9.2 K).

PLOT 10: Visualization showing the effect of quantity of alkaline earth metals on its constituting superconductor's critical temperature

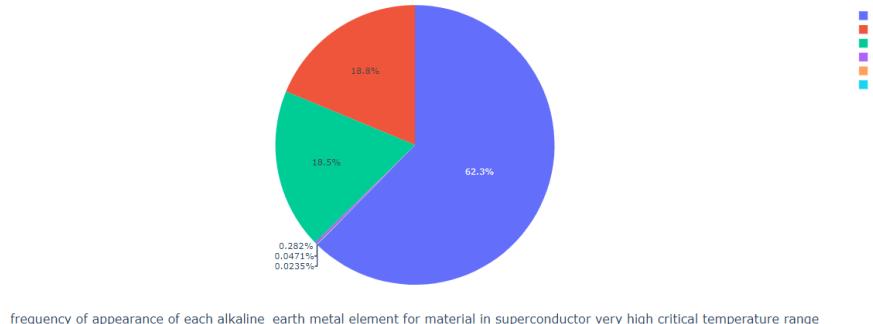


variation in choice and amount of each alkaline earth metal element for material in superconductor for a critical temperature range

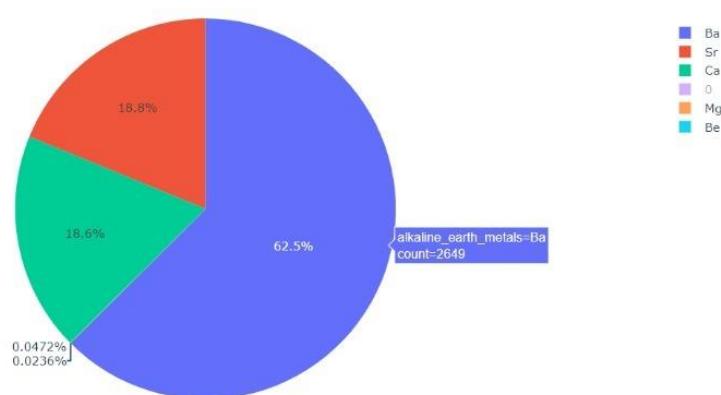


INFERENCES: Inference: Among the alkaline earth metals presence of Beryllium and Magnesium in excess indicates low Critical Temperature while presence of Barium, Strontium and Calcium in low proportions indicate moderate to high temperatures.

PLOT 11: Interactive pie chart showing the proportion in which how frequently alkaline earth metals are present among all superconductor materials that show very high critical temperatures



frequency of appearance of each alkaline_earth metal element for material in superconductor very high critical temperature range



frequency of appearance of each alkaline_earth metal element for material in superconductor very high critical temperature range

INFERENCES: Among all alkaline earth metals Barium has the most representation in the chemical formula of superconducting materials followed by Strontium and Calcium.

REVIEW 3

We have used a dataset containing the different chemical properties of superconductors, and analyze these records to better understand any underlying trends. These trends, as presented in this dashboard, reveal certain interesting patterns about the composition and nature of superconductors.

Many industries use these superconductors in different applications. Depending on the specific use case, the environment conditions change. All superconductors may not be sustainable in these conditions.

We attempt to use this data to determine what are the most favorable properties for a superconductors, and how the composition and property varies in different environment conditions. This dashboard will present our findings in an organized and interactive manner, and can be used as a guide by any industry looking to employ the use of superconductors, catered to their use case.

HOME PAGE: The home page provides an overview of our project and the team details. The sidebar on this homepage is consistent, and is an interactive navigation tool allowing us to navigate between the different pages of our dashboard.

Menu

Superconductors - Interactive Dashboard

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Material Visualization 4

Data Visualization Project: CSE-3020

Group 23

Mayukh Mondal: 20BCT0133

Rajarshi Saha: 20BCT0163

Parth Chaudhary: 15BCE2044

We explore the different chemical properties of superconductors, and analyze these records to better understand any underlying trends. These trends, as presented in this dashboard, reveal certain interesting patterns about the composition and nature of superconductors.

We have made use of the Superconductors Dataset from the UCI Machine Learning Repository. It is sourced from:

Hamidieh, Kam, A data-driven statistical model for predicting the critical temperature of a superconductor, Computational Materials Science, Volume 154, November 2018, Pages 346-354.

PROPERTY VISUALIZATION 1:

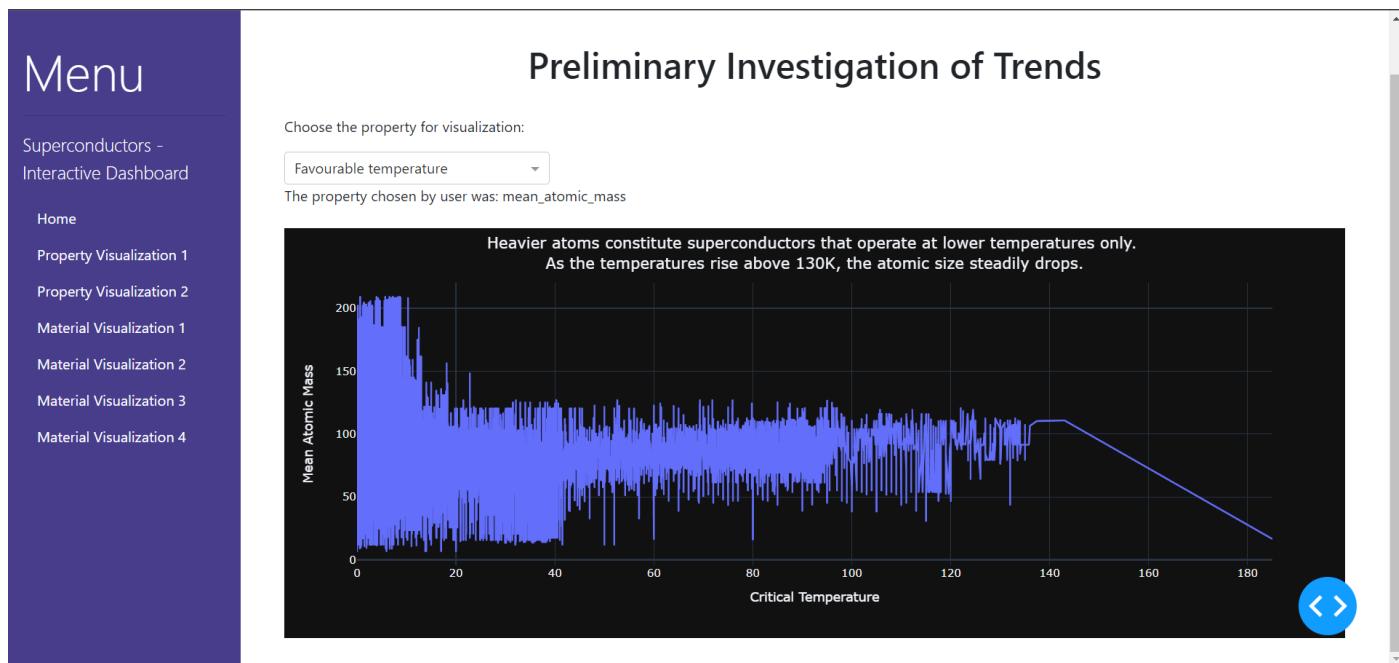
First, to get an overview of the data, we conduct a preliminary investigation of the different properties available to us. This would allow us to make some conclusions about the underlying trends in properties, and also reveal any anomalies.

We have implemented a drop-down menu, which allows us to choose between the different properties. Once chosen, that plot is visualized, and the plot title displays the conclusion drawn from that particular plot.

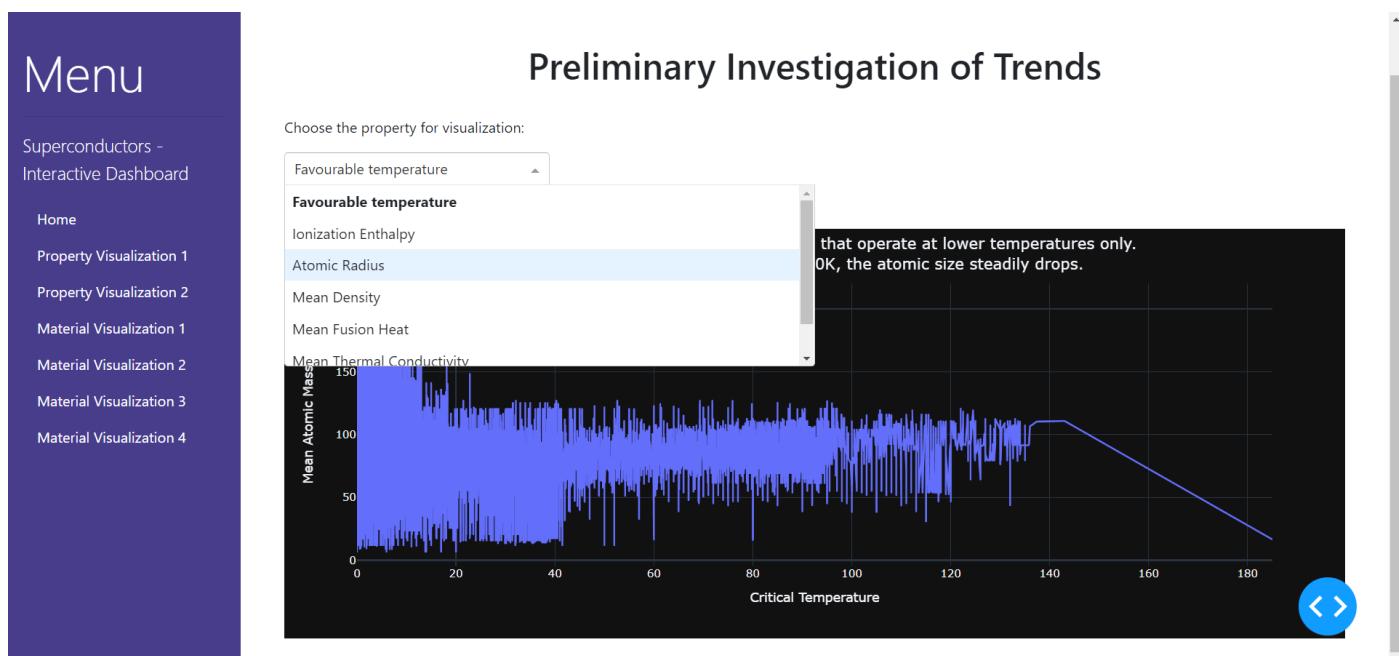
The main utility of these plots were that they allowed us to conclude that dividing the superconductors into elemental classes would definitely reveal distinctive patterns in their properties, which we have implemented in the Material Visualization plots.

PROPERTY CHOSEN: Favourable temperature

CONCLUSION: Heavier atoms constitute superconductors that operate at lower temperatures only. As the temperatures rise above 130K, the atomic mass steadily drops.



We see here, the different properties available to us from the drop-down menu, which is the main interactivity feature in this page of the dashboard.



PROPERTY CHOSEN: Atomic Radius

CONCLUSION: Larger atoms constitute superconductors that operate at lower temperatures only. As the temperatures rise above 130K, the atomic size steadily drops.

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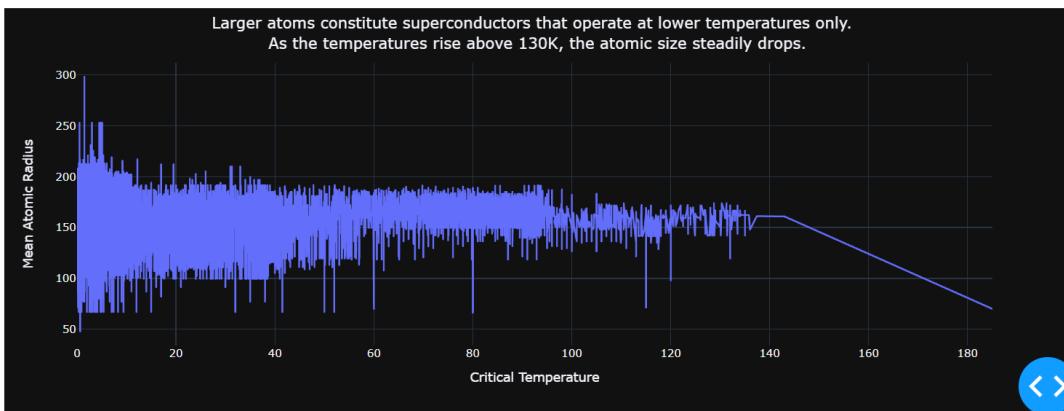
Material Visualization 4

Preliminary Investigation of Trends

Choose the property for visualization:

Atomic Radius

The property chosen by user was: mean_atomic_radius



PROPERTY CHOSEN: Mean Thermal Conductivity

CONCLUSION: Thermal conductivity decreases with rise in critical temperature. This is consistent with the trends in electron affinity and first ionization enthalpy

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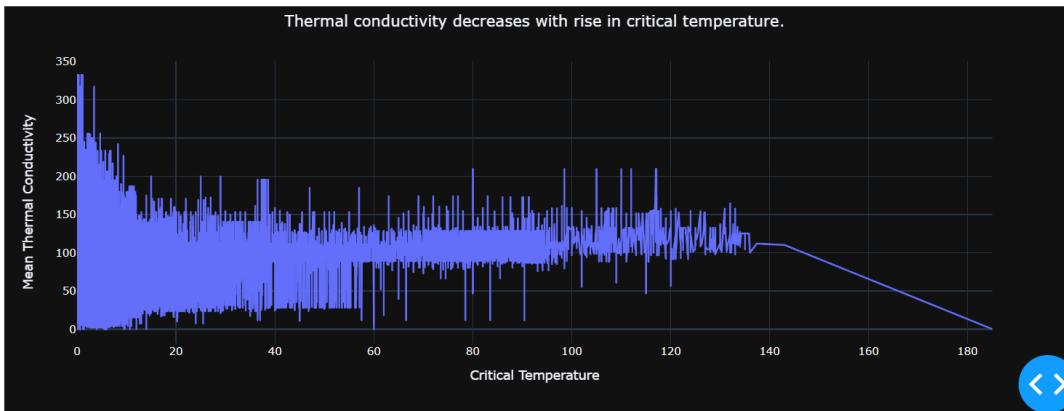
Material Visualization 4

Preliminary Investigation of Trends

Choose the property for visualization:

Mean Thermal Conductivity

The property chosen by user was: mean_ThermalConductivity



PROPERTY CHOSEN: Mean Valence

CONCLUSION: Valence decreases slightly, before increasing again. Transition metals, usually having a high valence, are therefore most likely to appear on either ends of this critical temperature spectrum with respect to mean valence.

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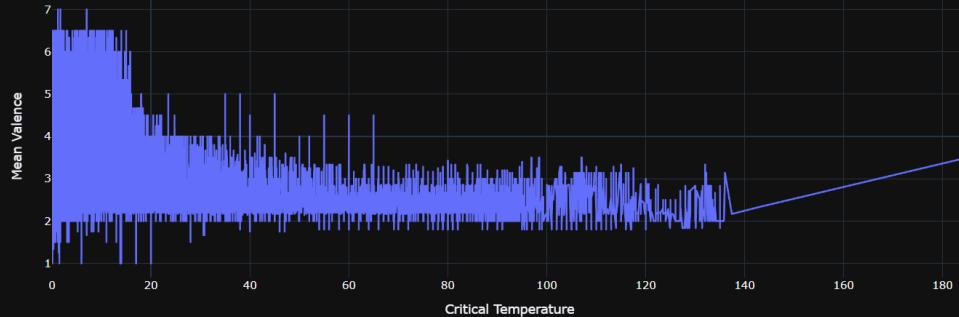
Preliminary Investigation of Trends

Choose the property for visualization:

Mean Valence

The property chosen by user was: mean_Valence

Valence decreases slightly, before increasing again.



PROPERTY VISUALIZATION 2:

We attempt to quantify the contribution of each attribute to the trend in the target. We plot a correlation matrix using Kendall's rank correlation coefficient method, which is a statistical method to measure the degree of ordinal association between two measured quantities. Thus, we obtain the strength of dependence of each property on critical temperature, obtained via Kendall's rank correlation coefficient method. This gives us a list of 8 most dominant properties, that are the most responsive to changes in critical temperature.

PROPERTY CHOSEN: Range of Thermal Conductivity

CONCLUSION: Thermal conductivity shows an almost linear increase, consistent with the positive correlation coefficient obtained. We also notice the high concentration of thermal conductivities in the (399.8 400.0] quantile. We can conclude most materials possessing thermal conductivities in this range are superconductors.

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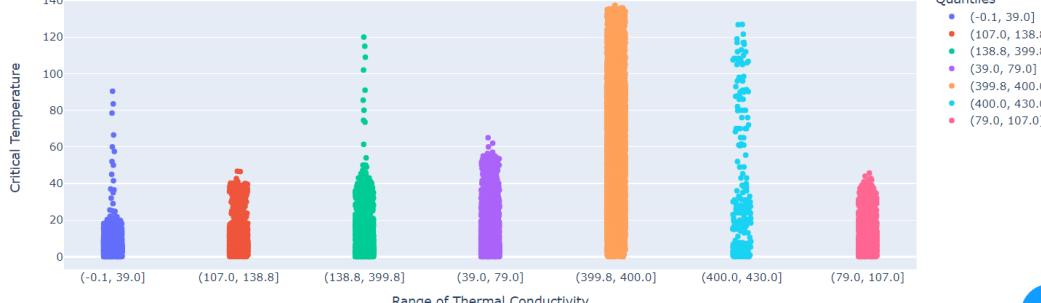
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Analysis of the Most Dominant Properties

Range of Thermal Conductivity

The property chosen by user was: range_ThermalConductivity

Thermal conductivity shows an almost linear increase, consistent with the positive correlation coefficient obtained.
We also notice the high concentration of thermal conductivities in the (399.8 400.0] quantile.

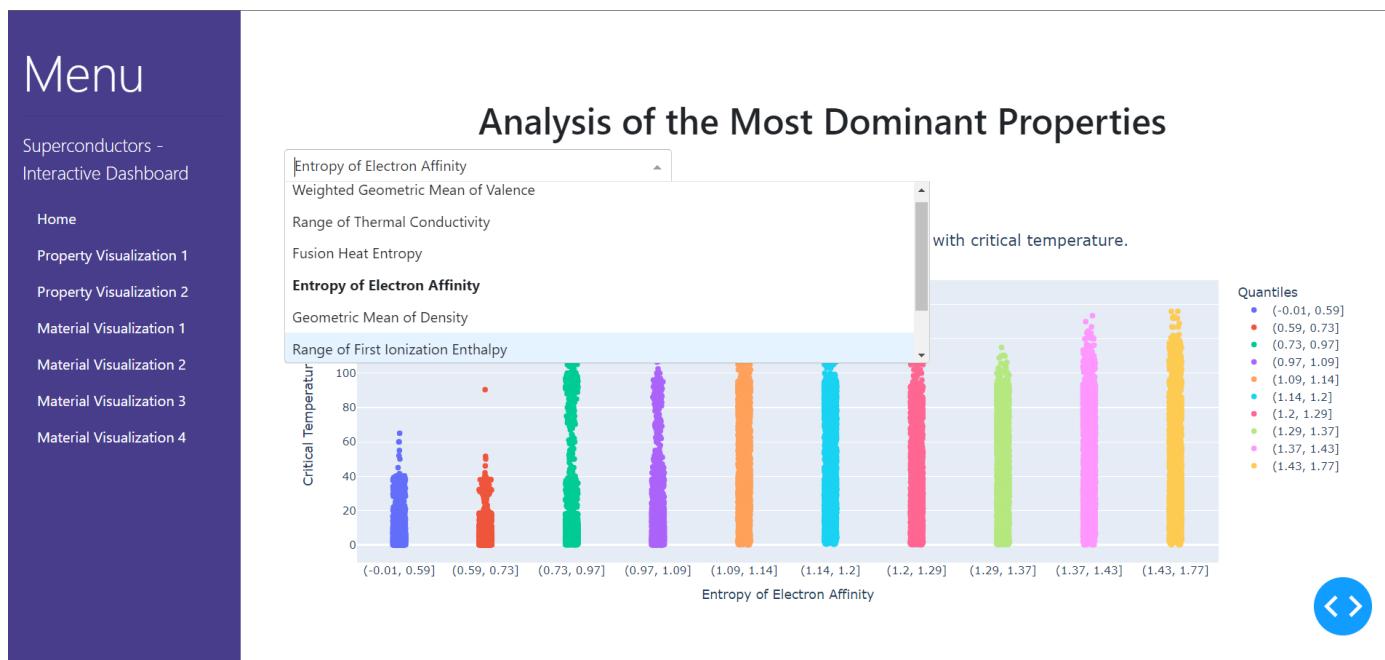


Quantiles

- (-0.1, 39.0]
- (107.0, 138.8]
- (138.8, 399.8]
- (39.0, 79.0]
- (399.8, 400.0]
- (400.0, 430.0]
- (79.0, 107.0]

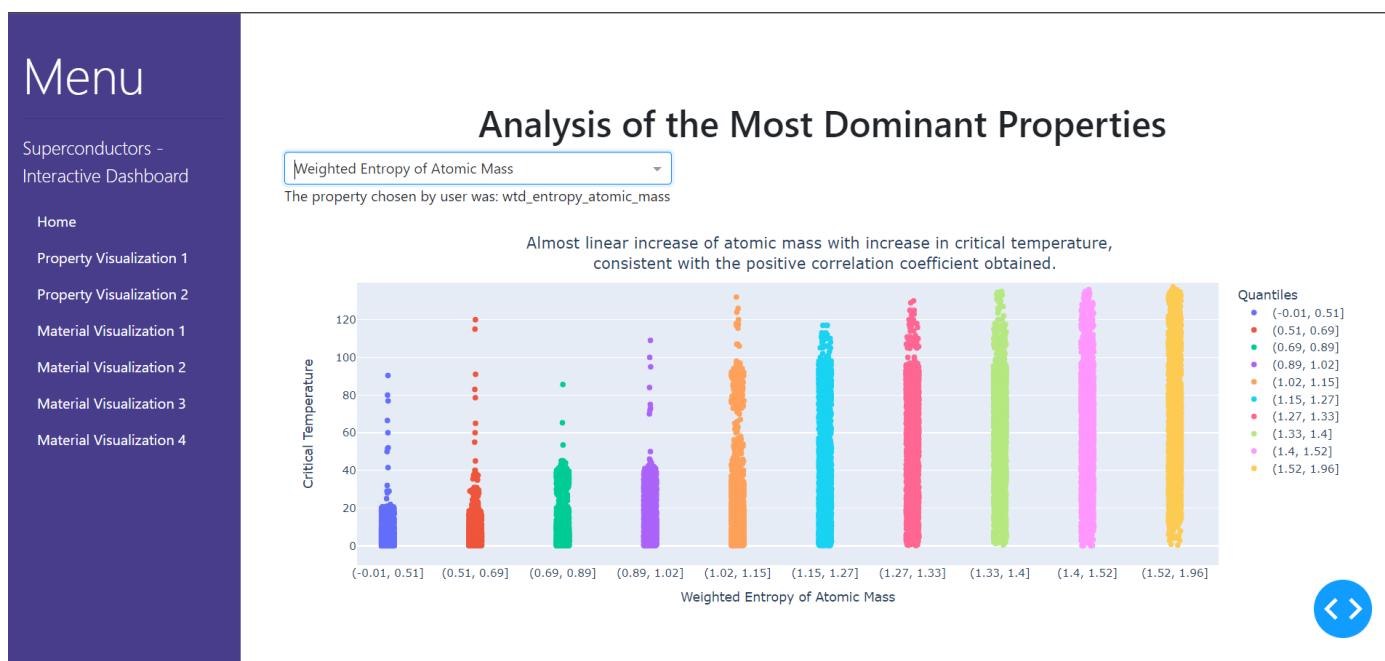


Here we see the implementation of the drop-down menu, and the list of most dominant properties out of which we can choose one at a time for visualization. We look for trends in the distribution of critical temperature in different property quantiles of the superconductors.



PROPERTY CHOSEN: Weighted Entropy of Atomic Mass

CONCLUSION: Almost linear increase of atomic size with increase in critical temperature, consistent with the positive correlation coefficient obtained.



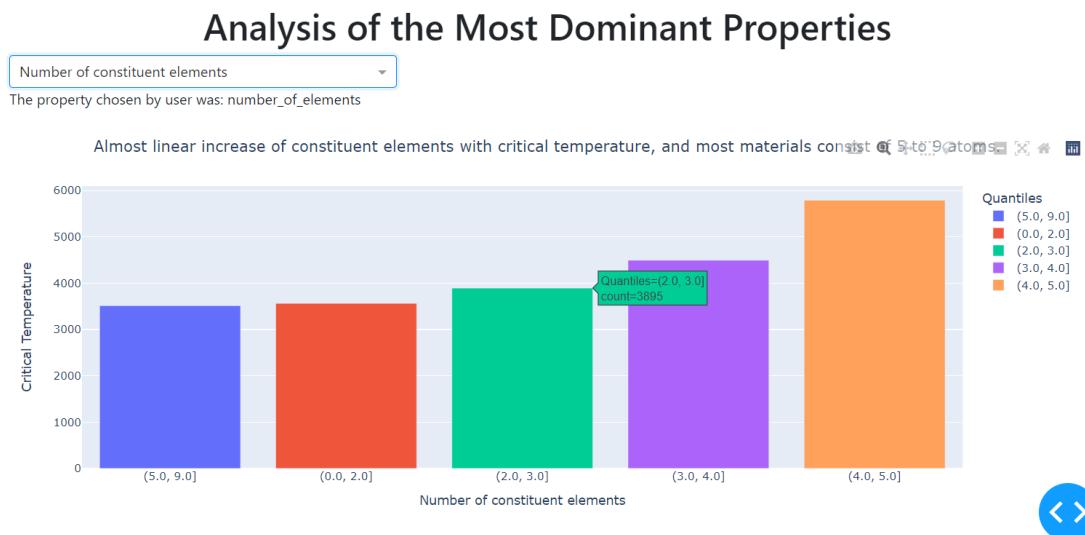
PROPERTY CHOSEN: Number of constituent elements

CONCLUSION: Almost linear increase of constituent elements with critical temperature, and most materials consist of 5 to 9 atoms.

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Now that we have shortlisted the most dominant properties and also visualized them, we can make the following important inferences from our trends in properties of the superconductors:

- There is a clear difference in the behaviour of superconductors having elements from different periodic classes.
- Within each of these classes, there is further difference in behaviour in different quantiles of the data

MATERIAL VISUALIZATION 1:

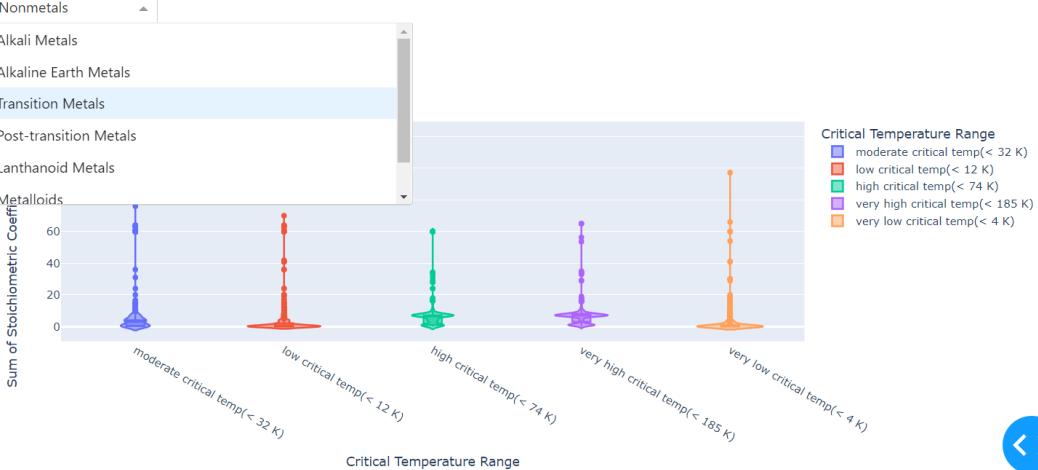
We answer the question of how the different elemental classes affect the critical temperature of superconductors by segregating these superconductors in different temperature ranges of critical temperature. We attempt to show how stoichiometric coefficients of each element groups present in a superconductor affect the critical temperature region in which the material behaves superconductor properties.

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Visualizing the presence of different elemental series in different critical temperature ranges

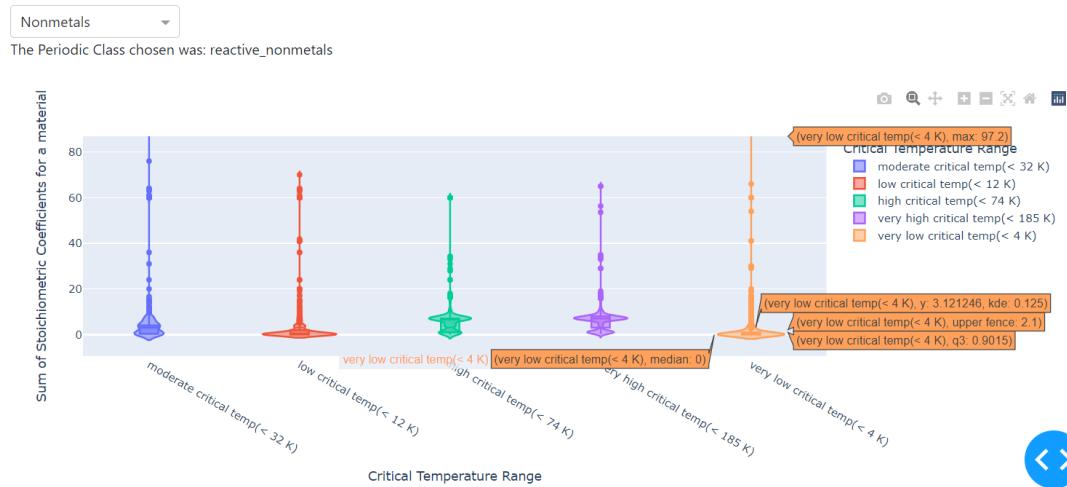


PERIODIC CLASS: Non-metals

We see that there is a much larger presence of non-metals with the critical temperature 0 – 12 K that is, low and very low critical temperatures. Also, we see that in very low and moderate critical temperatures, there also tends to be high variability in the number of constituent elements in the superconductor.



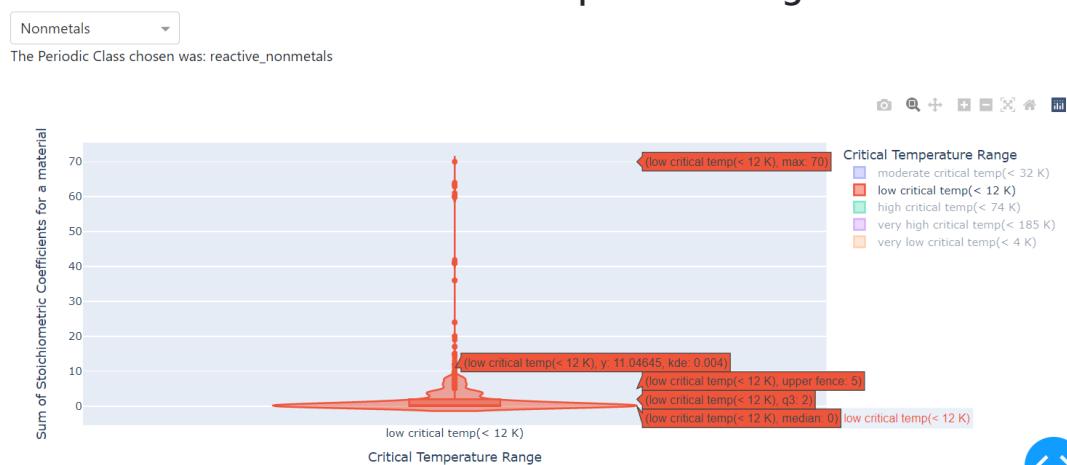
Visualizing the presence of different elemental series in different critical temperature ranges



Here, we can infer those nonmetals must be present in very tiny proportions (<2) for the superconductor to have low critical temperature while to reach high temperatures, majority of superconducting materials are present in higher proportions (>5).



Visualizing the presence of different elemental series in different critical temperature ranges



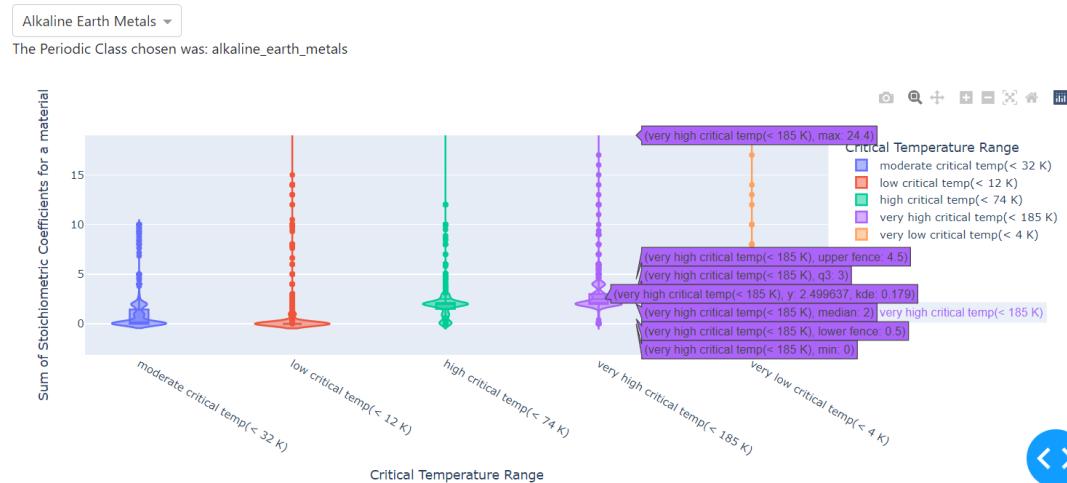
PERIODIC CLASS: Alkaline earth metals

We notice a high variability in the superconductors' stoichiometries in this elemental class with superconductors containing very low proportions of them exhibiting very low to moderate critical temperatures while high critical ranges beginning to show for materials with excess proportions of those.

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Visualizing the presence of different elemental series in different critical temperature ranges



MATERIAL VISUALIZATION 2:

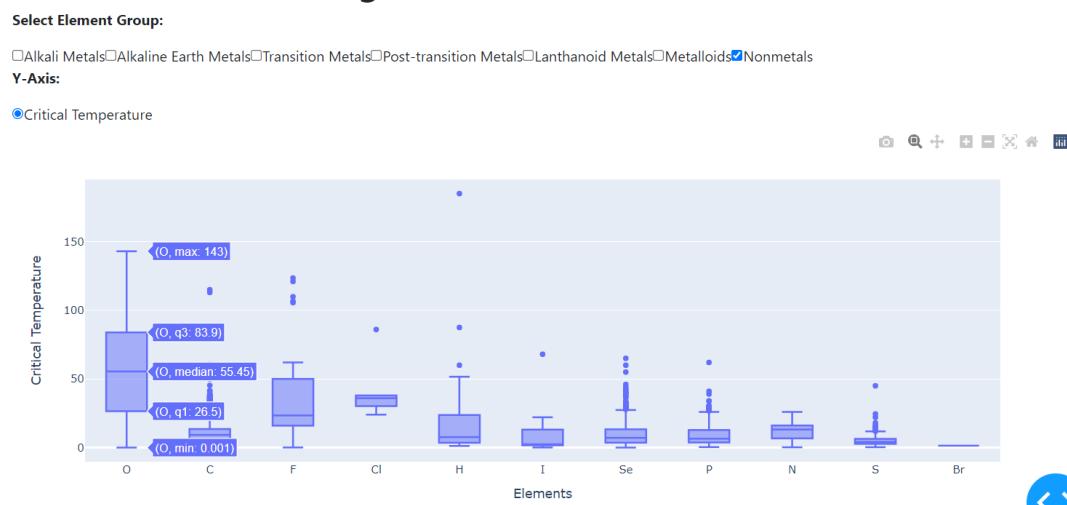
This visualization has been devised to observe distribution of critical temperature for materials containing a particular element from element groups selected in the checkboxes. At a time, one or more checkboxes can be selected, and we are able to visualize all the elements in that elemental class at the same time. It allows for clear comparison in the differences in critical temperature with the change in constituent materials.

In the plot below, we see those superconducting materials containing Oxygen (median temp: 55.45 K) exhibit higher critical temperatures than those containing Carbon (median temp: 9.2 K).

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Distribution of critical temperatures of superconductors according to their constituent materials



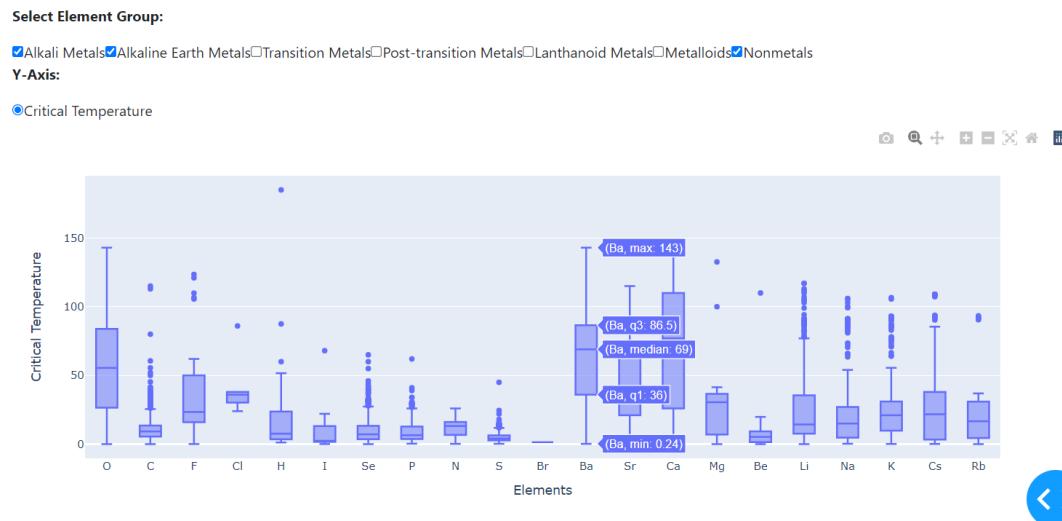
Below, we have selected alkali metals, alkaline earth metals and non-metals. As stated before, we are clearly able to see the difference in critical temperature distributions of these different elemental series, as well as notice the trends in each of these series as well.

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Distribution of critical temperatures of superconductors according to their constituent materials



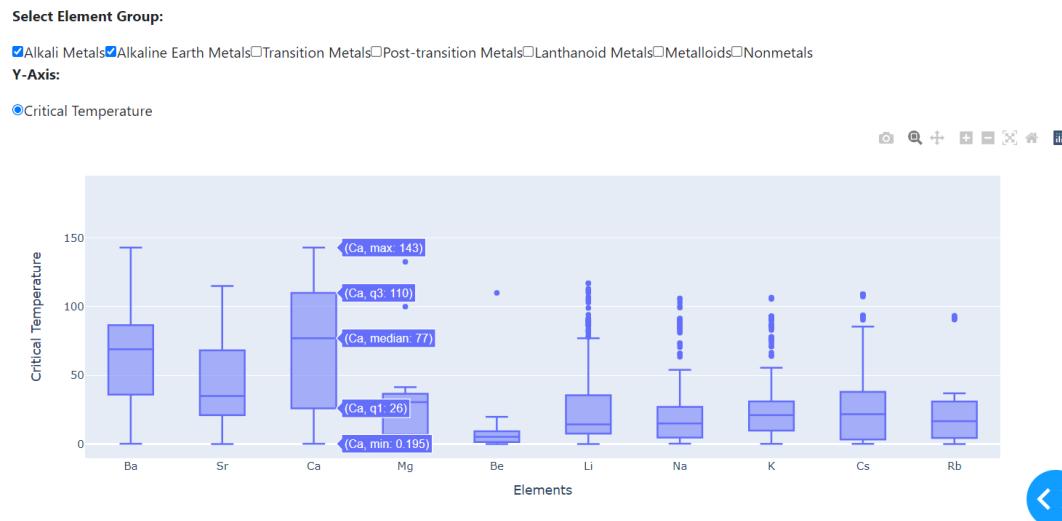
Between alkali metals and alkaline earth metals, we see that the mean, median and minimum critical temperature is significantly higher than that of superconductors containing alkali metals.

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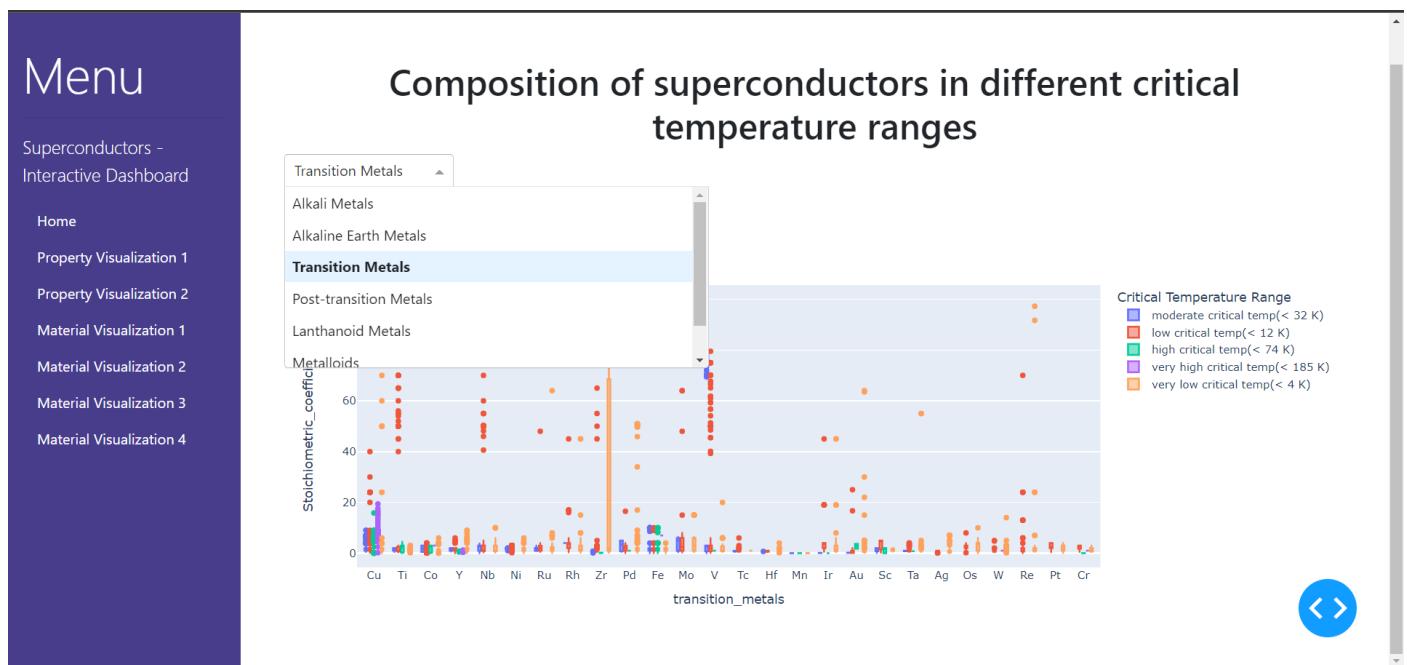
Distribution of critical temperatures of superconductors according to their constituent materials



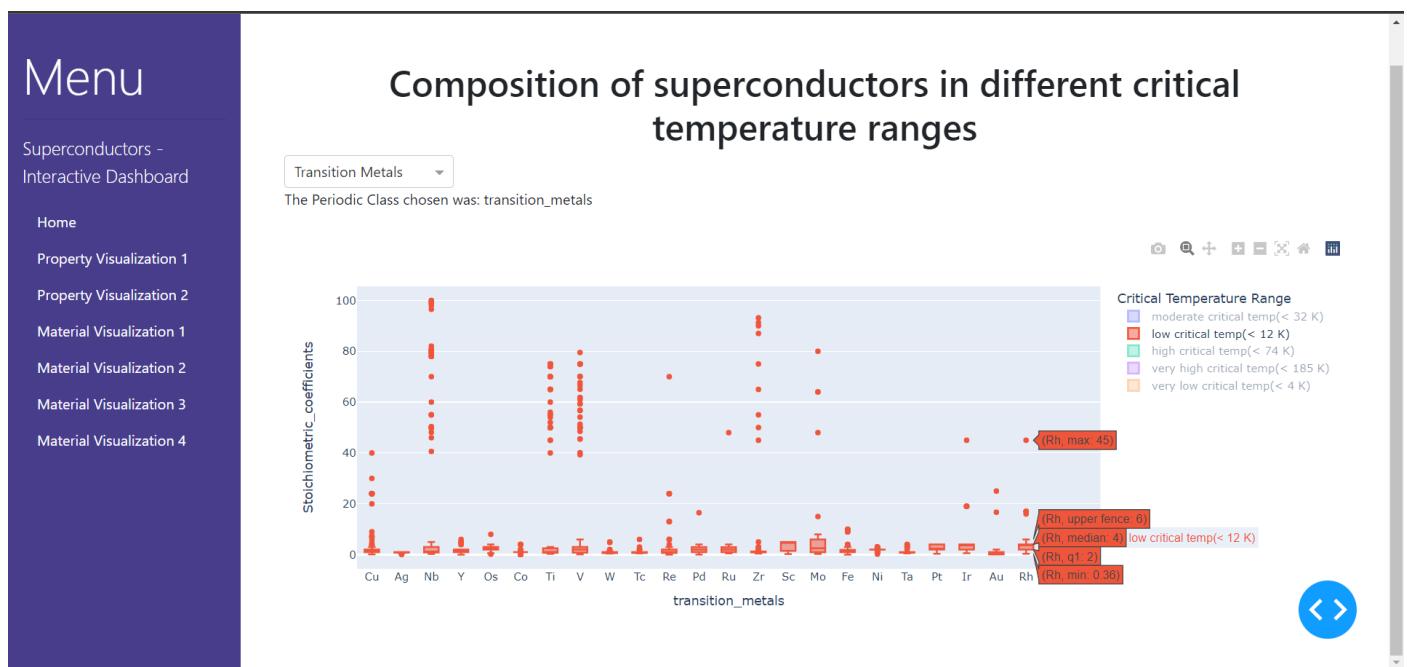
MATERIAL VISUALIZATION 3:

In this visualization we attempt to show the effect of quantity of elements from the element group selected in the dropdown menu on its constituting superconductor's critical temperature.

This is a more quantitative analysis, in direct contrast to the more qualitative analysis in Material Visualization 2.



Below for transition metals, we see that Niobium, Titanium, Vanadium and Zirconium have highly variable behaviour, whereas the others display pretty consistent behaviour. For example, Rhodium has very few outliers and displays low stoichiometric coefficients in the low critical temperature range.



For alkaline earth metals, we see that in the moderate critical temperature range, a superconductor containing Calcium is most probable to have the highest stoichiometric coefficients, since its distribution has the highest median. It also has a high variability, with the maximum displayed value as 10.

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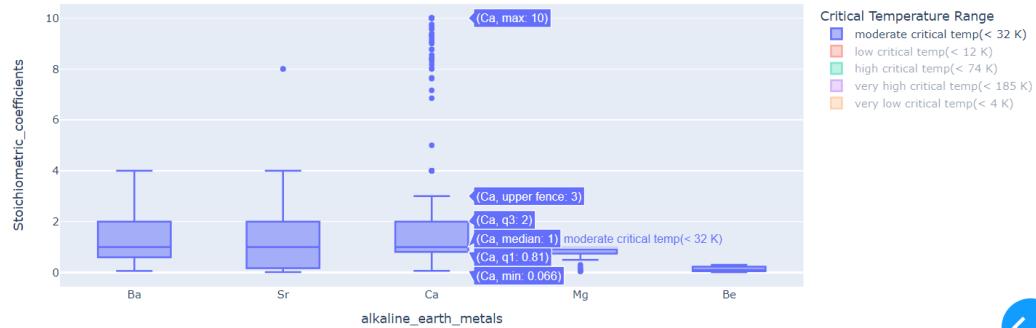
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Composition of superconductors in different critical temperature ranges

Alkaline Earth Metals ▾

The Periodic Class chosen was: alkaline_earth_metals



MATERIAL VISUALIZATION 4:

In this final visualization for our dashboard, we sum up all our observations. This page of the dashboard features an interactive pie chart showing the proportion in which elements of a group (selected from first dropdown) are present among all superconductor materials that show critical temperatures in a particular range (selected from second dropdown) either quantitatively/frequently (selected from third dropdown).

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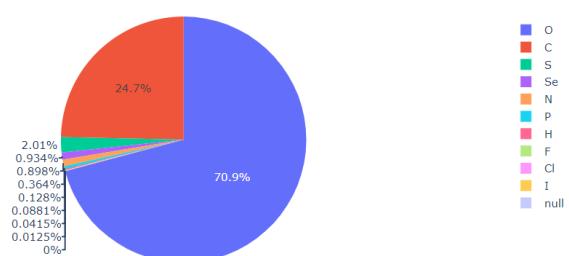
Overview of Superconducting Materials

Choose the desired specification to generate the chart:

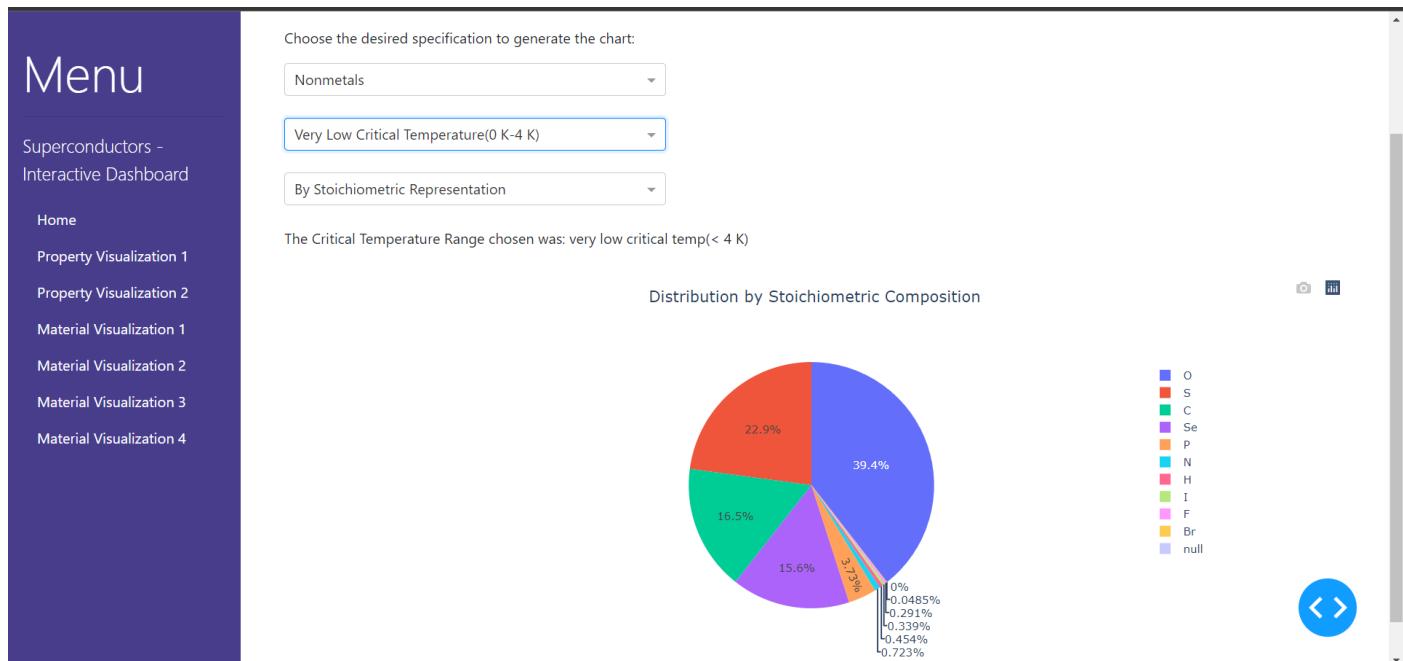
Nonmetals

- Alkaline Earth Metals
- Transition Metals
- Post-transition Metals
- Lanthanoid Metals
- Metalloids
- Nonmetals**

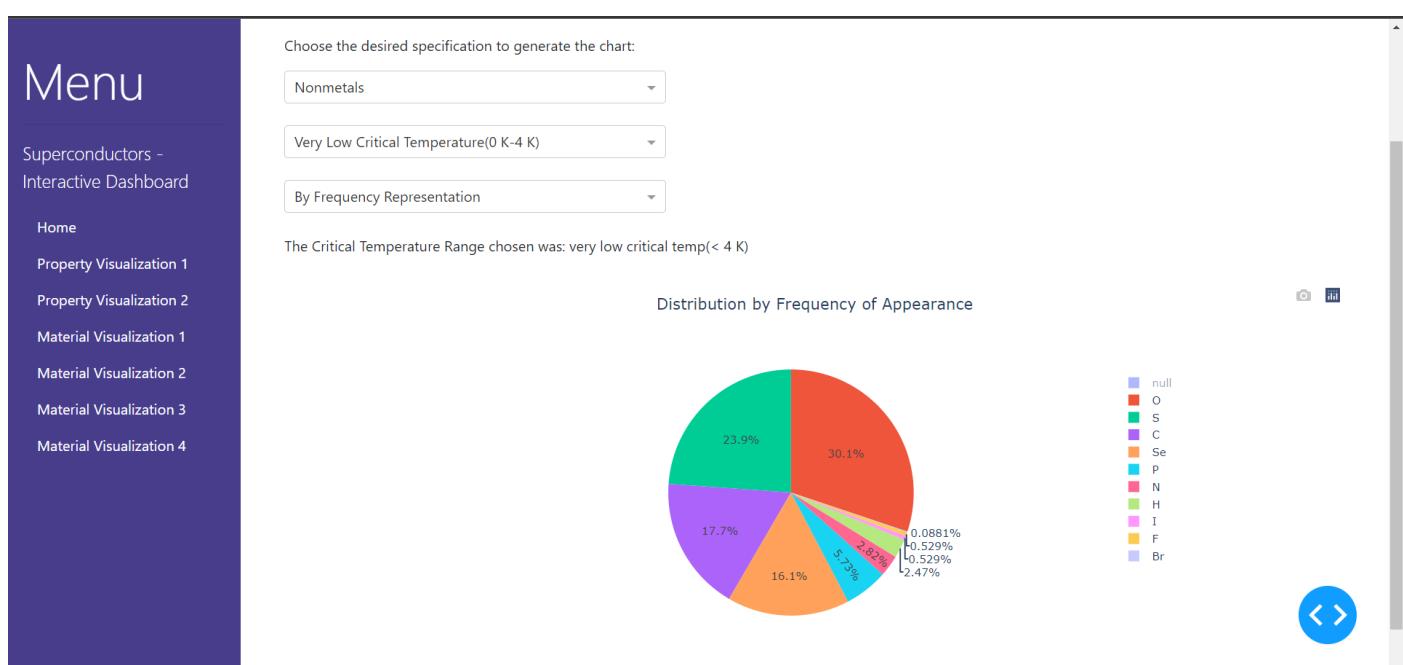
Distribution by Stoichiometric Composition



We can see that this interactive pie chart shows the proportion in which non-metals are present among all superconductor materials that show very low critical temperatures quantitatively.



Here this interactive pie chart shows the proportion in which how frequently non-metals are present among all superconductor materials that show very low critical temperatures.



This chart shows the proportion in which alkaline earth metals are present among all superconductor materials that show very high critical temperatures quantitatively.

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Choose the desired specification to generate the chart:

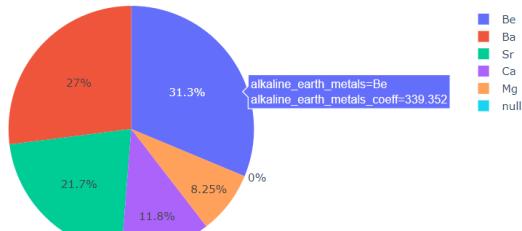
Alkaline Earth Metals

Very Low Critical Temperature(0 K-4 K)

By Stoichiometric Representation

The Critical Temperature Range chosen was: very low critical temp(< 4 K)

Distribution by Stoichiometric Composition



Video presentation (Review 2 & 3): <https://www.youtube.com/watch?v=Ua47-FAIEzc>