Predicting Mercury’s elemental composition from Albedo with MESSENGER Data

In [6]:

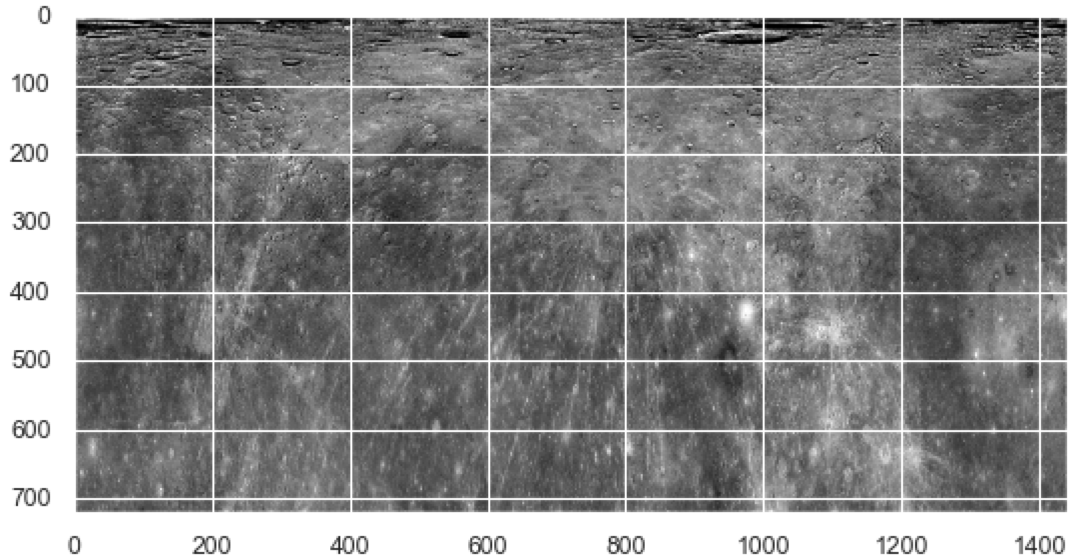
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import matplotlib as mpl
import warnings
warnings.filterwarnings('ignore')
from matplotlib.pyplot import figure
mpl.style.use('classic')
# %matplotlib inline

# from sklearn import metrics
sns.set()
```

In [7]:

```
#Step 1 - > Converting all the data frames into Numpy Matrix

# 720*1440
Mercury_top = pd.read_csv("mercury-albedo-top-half.png.csv",header=None);
Mercury_bottom = pd.read_csv("mercury-albedo-resized-bottom-half.png.csv",header=None);

Al =  pd.read_csv("alsimap_smooth_032015.png.csv",header=None);
Mg =  pd.read_csv("mgsimap_smooth_032015.png.csv",header=None);
Ca  =  pd.read_csv("casimap_smooth_032015.png.csv",header=None);
S =  pd.read_csv("ssimap_smooth_032015.png.csv",header=None);
Fe =  pd.read_csv("fesimap_smooth_032015.png.csv",header=None);



mercury_top = Mercury_top.to_numpy()
mercury_bottom = Mercury_bottom.to_numpy()

al = Al.to_numpy()
fe = Fe.to_numpy()
mg = Mg.to_numpy()
s = S.to_numpy()
ca = Ca.to_numpy()




flat_fe = fe.flatten()
flat_al = al.flatten()
flat_mg = mg.flatten()
flat_s = s.flatten()
flat_ca = ca.flatten()

flat_albedo = mercury_top.flatten()
data_train = {

        'Albedo':flat_albedo,'Fe':flat_fe,
        'Al':flat_al,'Mg':flat_mg,'S':flat_s,'Ca':flat_ca
}
```

In [8]:

```
#Plotting to the original to check if the above conversion of successful

plt.imshow(mercury_top, cmap="gray")
plt.show()
```



In [9]:

```
train =  pd.DataFrame(data= data_train)
```

In [10]:

```
#Step 3-> Lets do some EDA

train.head()
```

Out[10]:

	Albedo	Fe	Al	Mg	S	Ca
0	0.486275	0.0	0.0	0.0	0.0	0.0
1	0.498039	0.0	0.0	0.0	0.0	0.0
2	0.521569	0.0	0.0	0.0	0.0	0.0
3	0.529412	0.0	0.0	0.0	0.0	0.0
4	0.541176	0.0	0.0	0.0	0.0	0.0

In [11]:

```
#Lets get some insights about the data using info() and describe() methods.

train.describe()
```

Out[11]:

	Albedo	Fe	Al	Mg	S	Ca
count	1.036800e+06	1.036800e+06	1.036800e+06	1.036800e+06	1.036800e+06	1.036800e+06
mean	4.144590e-01	3.138895e-01	7.510351e-01	5.303197e-01	3.859588e-01	4.086300e-01
std	1.165033e-01	2.891811e-01	1.989632e-01	1.432387e-01	2.304556e-01	2.254984e-01
min	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
25%	3.372549e-01	0.000000e+00	7.137255e-01	4.980392e-01	3.529412e-01	4.274510e-01
50%	4.039216e-01	4.549020e-01	8.039216e-01	5.411765e-01	4.509804e-01	4.941176e-01
75%	4.862745e-01	5.607843e-01	8.745098e-01	5.803922e-01	5.098040e-01	5.333334e-01
max	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00

In [12]:

```
train.info()
```

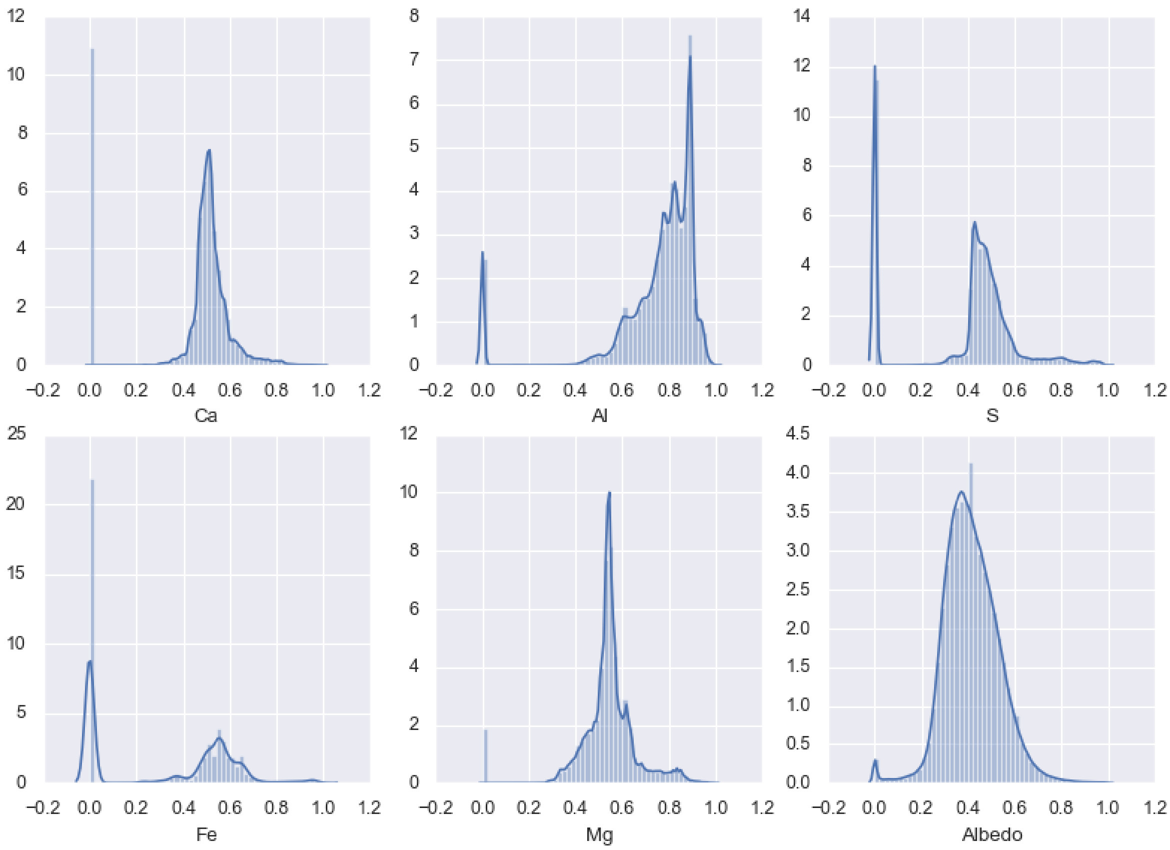
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1036800 entries, 0 to 1036799
Data columns (total 6 columns):
 #   Column  Non-Null Count    Dtype  
---  ------  --------------    -----  
 0   Albedo  1036800 non-null  float64
 1   Fe      1036800 non-null  float64
 2   Al      1036800 non-null  float64
 3   Mg      1036800 non-null  float64
 4   S       1036800 non-null  float64
 5   Ca      1036800 non-null  float64
dtypes: float64(6)
memory usage: 47.5 MB
```

In [13]:

```
#Let's visualize the chemical compositions and Albedo data


figure(num=None, figsize=(12, 8), dpi=80, facecolor='w', edgecolor='k')

plt.subplot(2, 3, 1)
sns.distplot(train['Ca'])

plt.subplot(2, 3, 2)
sns.distplot(train['Al'])

plt.subplot(2, 3, 3)
sns.distplot(train['S'])

plt.subplot(2, 3, 4)
sns.distplot(train['Fe'])

plt.subplot(2, 3, 5)
sns.distplot(train['Mg'])

plt.subplot(2, 3, 6)
sns.distplot(train['Albedo'])
```

Out[13]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x2827916fc08>
```



In [14]:

```
#Ingsights from the plots above
#Almost all of the element variables have high no. of zeros indicating missing data. Lets p

print("No. of zeros in Al -> ",np.count_nonzero(flat_al==0))
print("No. of zeros in Mg -> ",np.count_nonzero(flat_mg==0))
print("No. of zeros in Fe -> ",np.count_nonzero(flat_fe==0))
print("No. of zeros in S -> ",np.count_nonzero(flat_s==0))
print("No. of zeros in Ca -> ",np.count_nonzero(flat_ca==0))
```

```
No. of zeros in Al ->  50809
No. of zeros in Mg ->  39303
No. of zeros in Fe ->  452442
No. of zeros in S ->  238107
No. of zeros in Ca ->  226264
```

Fixing Zeros

The most intutive way to mix zeros will be using KNN(K-Nearest Neighbours Regressor) to predict the missing region using the data of nearby regions.

Replacing zeros with nan

In [28]:

```
cols = ["Fe","Al","Mg","S","Ca"]
train[cols] = train[cols].astype(object)

#Creating the train data as the the non-missing values and test data the region of missing


df_fe = train[['Albedo','Fe']]
train_df_fe = df_fe.dropna()
test_df_fe = train[train['Fe'].isnull()]

df_al = train[['Albedo','Al']]
train_df_al = df_al.dropna()
test_df_al = train[train['Al'].isnull()]

df_mg = train[['Albedo','Mg']]
train_df_mg = df_mg.dropna()
test_df_mg = train[train['Mg'].isnull()]

df_s = train[['Albedo','S']]
train_df_s = df_s.dropna()
test_df_s = train[train['S'].isnull()]

df_ca = train[['Albedo','Ca']]
train_df_ca = df_ca.dropna()
test_df_ca = train[train['Ca'].isnull()]
```

In [29]:

```
#Note - Many instances of using different values of k have been done but all have not been

from sklearn import metrics
from sklearn.neighbors import KNeighborsRegressor
```

In [55]:

```
error_rate=[]
for i in range(16,30,5):

    knn = KNeighborsRegressor(n_neighbors=i,metric='euclidean')
    knn.fit(X_train,y_train)
    pred_i = knn.predict(X_train)
    print('k=>',i,' error',metrics.mean_squared_error(pred_i,y_train))
    error_rate.append(metrics.mean_squared_error(pred_i,y_train))
```

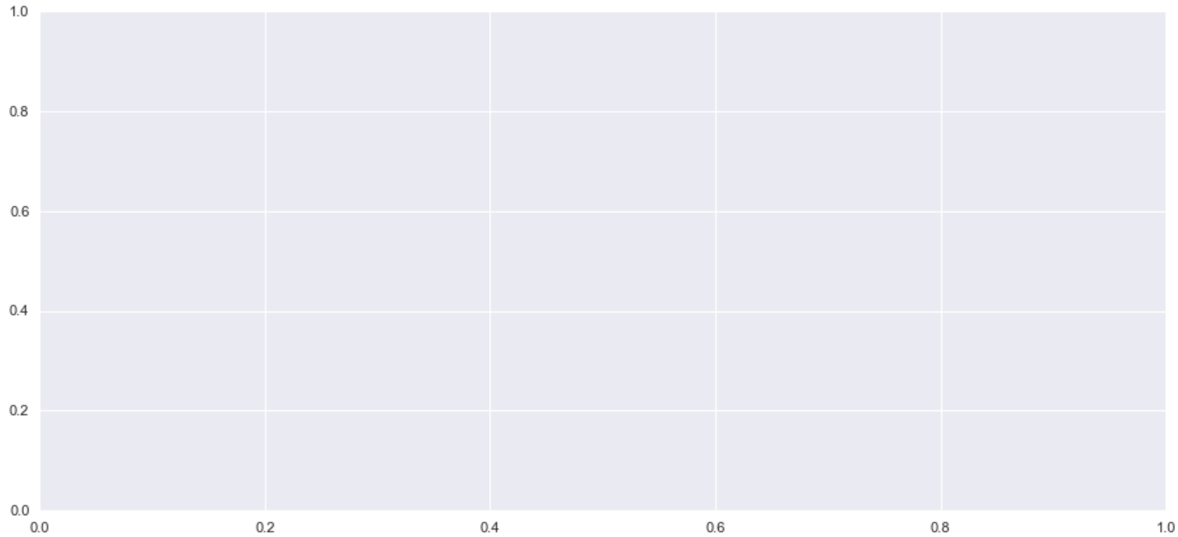
```
k=> 16  error 0.08812882802493324
k=> 21  error 0.08724238090342852
k=> 26  error 0.08679706969215625
```

In [57]:

```
plot_x = [1,6,11,16,16,21,26,30,40,50,60]

plt.figure(figsize=(14,6))
plt.plot(plot_x,error_rate,color='blue', linestyle='dashed', marker='o',
         markerfacecolor='red', markersize=10)
plt.title('Error Rate vs. K Value')
plt.xlabel('K')
plt.ylabel('Error Rate')
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-57-b3bdda1e6be1> in <module>
      3 plt.figure(figsize=(14,6))
      4 plt.plot(plot_x,error_rate,color='blue', linestyle='dashed', marker
='o',
----> 5          markerfacecolor='red', markersize=10)
      6 plt.title('Error Rate vs. K Value')
      7 plt.xlabel('K')

E:\anxe\lib\site-packages\matplotlib\pyplot.py in plot(scalex, scaley, data,
*args, **kwargs)
   2794     return gca().plot(
   2795         *args, scalex=scalex, scaley=scaley, **({"data": data} if da
ta
-> 2796         is not None else {}), **kwargs)
   2797
   2798

E:\anxe\lib\site-packages\matplotlib\axes\_axes.py in plot(self, scalex, sca
ley, data, *args, **kwargs)
   1663         """
   1664         kwargs = cbook.normalize_kwargs(kwargs, mlines.Line2D._alias
_map)
-> 1665         lines = [*self._get_lines(*args, data=data, **kwargs)]
   1666         for line in lines:
   1667             self.add_line(line)

E:\anxe\lib\site-packages\matplotlib\axes\_base.py in __call__(self, *args,
 **kwargs)
    223                 this += args[0],
    224                 args = args[1:]
--> 225             yield from self._plot_args(this, kwargs)
    226
    227     def get_next_color(self):

E:\anxe\lib\site-packages\matplotlib\axes\_base.py in _plot_args(self, tup,
 kwargs)
    389             x, y = index_of(tup[-1])
    390
--> 391         x, y = self._xy_from_xy(x, y)
    392
    393         if self.command == 'plot':

E:\anxe\lib\site-packages\matplotlib\axes\_base.py in _xy_from_xy(self, x,
 y)
    268         if x.shape[0] != y.shape[0]:
    269             raise ValueError("x and y must have same first dimensio
n, but "
--> 270                              "have shapes {} and {}".format(x.shape,
```

```
y.shape))
    271         if x.ndim > 2 or y.ndim > 2:
    272             raise ValueError("x and y can be no greater than 2-D, bu
t have "

ValueError: x and y must have same first dimension, but have shapes (11,) an
d (3,)
```



In [34]:

```
# Fe
X_train =train_df_fe.drop('Fe',axis =1)
y_train = train_df_fe['Fe']
X_test = (test_df_fe['Albedo'].to_numpy()).reshape(test_df_fe['Albedo'].to_numpy().size,1)

knn = KNeighborsRegressor(n_neighbors=25)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
train.loc[train.Fe.isnull(), 'Fe'] = y_pred

# Al

X_train =train_df_al.drop('Al',axis =1)
y_train = train_df_al['Al']
X_test = (test_df_al['Albedo'].to_numpy()).reshape(test_df_al['Albedo'].to_numpy().size,1)


knn = KNeighborsRegressor(n_neighbors=25)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
train.loc[train.Al.isnull(), 'Al'] = y_pred

# Mg

X_train =train_df_mg.drop('Mg',axis =1)
y_train = train_df_mg['Mg']
X_test = (test_df_mg['Albedo'].to_numpy()).reshape(test_df_mg['Albedo'].to_numpy().size,1)

knn = KNeighborsRegressor(n_neighbors=25)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
train.loc[train.Mg.isnull(), 'Mg'] = y_pred

# S
X_train =train_df_s.drop('S',axis =1)
y_train = train_df_s['S']
X_test = (test_df_s['Albedo'].to_numpy()).reshape(test_df_s['Albedo'].to_numpy().size,1)

knn = KNeighborsRegressor(n_neighbors=25)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
train.loc[train.S.isnull(), 'S'] = y_pred


# Ca
X_train =train_df_ca.drop('Ca',axis =1)
y_train = train_df_ca['Ca']
X_test = (test_df_ca['Albedo'].to_numpy()).reshape(test_df_ca['Albedo'].to_numpy().size,1)

knn = KNeighborsRegressor(n_neighbors=25)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
train.loc[train.Ca.isnull(), 'Ca'] = y_pred
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-34-b7cdb7fa0dc1> in <module>
```

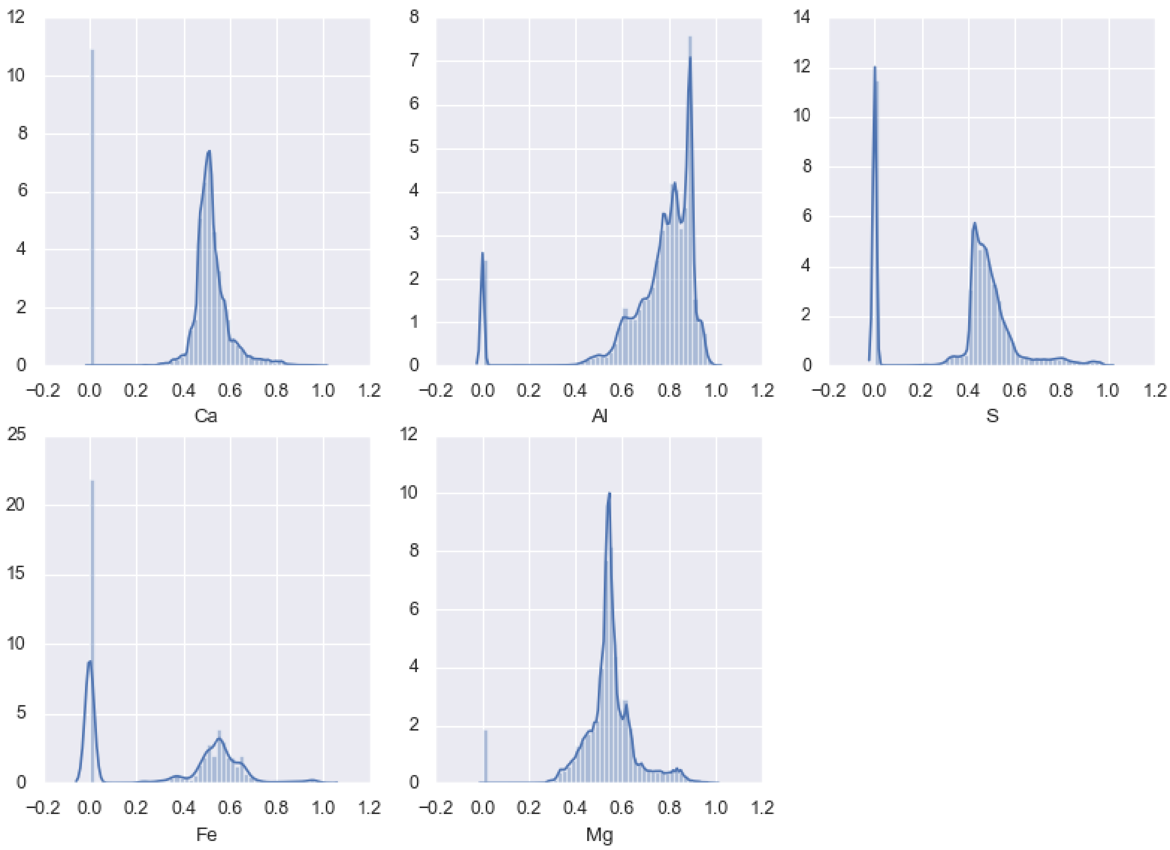
```
      6 knn = KNeighborsRegressor(n_neighbors=25)
      7 knn.fit(X_train, y_train)
----> 8 y_pred = knn.predict(X_test)
      9 train.loc[train.Fe.isnull(), 'Fe'] = y_pred
     10

E:\anxe\lib\site-packages\sklearn\neighbors\_regression.py in predict(sel
f, X)
    170             Target values
    171         """
--> 172         X = check_array(X, accept_sparse='csr')
    173
    174         neigh_dist, neigh_ind = self.kneighbors(X)

E:\anxe\lib\site-packages\sklearn\utils\validation.py in check_array(arra
y, accept_sparse, accept_large_sparse, dtype, order, copy, force_all_finit
e, ensure_2d, allow_nd, ensure_min_samples, ensure_min_features, warn_on_d
type, estimator)
    584                              " minimum of %d is required%s."
    585                              % (n_samples, array.shape, ensure_min
_samples,
--> 586                                 context))
    587
    588     if ensure_min_features > 0 and array.ndim == 2:

ValueError: Found array with 0 sample(s) (shape=(0, 1)) while a minimum of
1 is required.
```

In [21]:

```
figure(num=None, figsize=(12, 8), dpi=80, facecolor='w', edgecolor='k')

plt.subplot(2, 3, 1)
sns.distplot(train['Ca'])

plt.subplot(2, 3, 2)
sns.distplot(train['Al'])

plt.subplot(2, 3, 3)
sns.distplot(train['S'])

plt.subplot(2, 3, 4)
sns.distplot(train['Fe'])

plt.subplot(2, 3, 5)
sns.distplot(train['Mg'])
```

Out[21]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x28274dc8e48>
```



In [22]:

```
train.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1036800 entries, 0 to 1036799
Data columns (total 6 columns):
 #   Column  Non-Null Count    Dtype  
---  ------  --------------    -----  
 0   Albedo  1036800 non-null  float64
 1   Fe      1036800 non-null  float64
 2   Al      1036800 non-null  float64
 3   Mg      1036800 non-null  float64
 4   S       1036800 non-null  float64
 5   Ca      1036800 non-null  float64
dtypes: float64(6)
memory usage: 47.5 MB
```

In [23]:

```
train.describe()
```

Out[23]:

	Albedo	Fe	Al	Mg	S	Ca
count	1.036800e+06	1.036800e+06	1.036800e+06	1.036800e+06	1.036800e+06	1.036800e+06
mean	4.144590e-01	3.138895e-01	7.510351e-01	5.303197e-01	3.859588e-01	4.086300e-01
std	1.165033e-01	2.891811e-01	1.989632e-01	1.432387e-01	2.304556e-01	2.254984e-01
min	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
25%	3.372549e-01	0.000000e+00	7.137255e-01	4.980392e-01	3.529412e-01	4.274510e-01
50%	4.039216e-01	4.549020e-01	8.039216e-01	5.411765e-01	4.509804e-01	4.941176e-01
75%	4.862745e-01	5.607843e-01	8.745098e-01	5.803922e-01	5.098040e-01	5.333334e-01
max	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00	1.000000e+00

In [24]:

```
train.corr()
```

Out[24]:

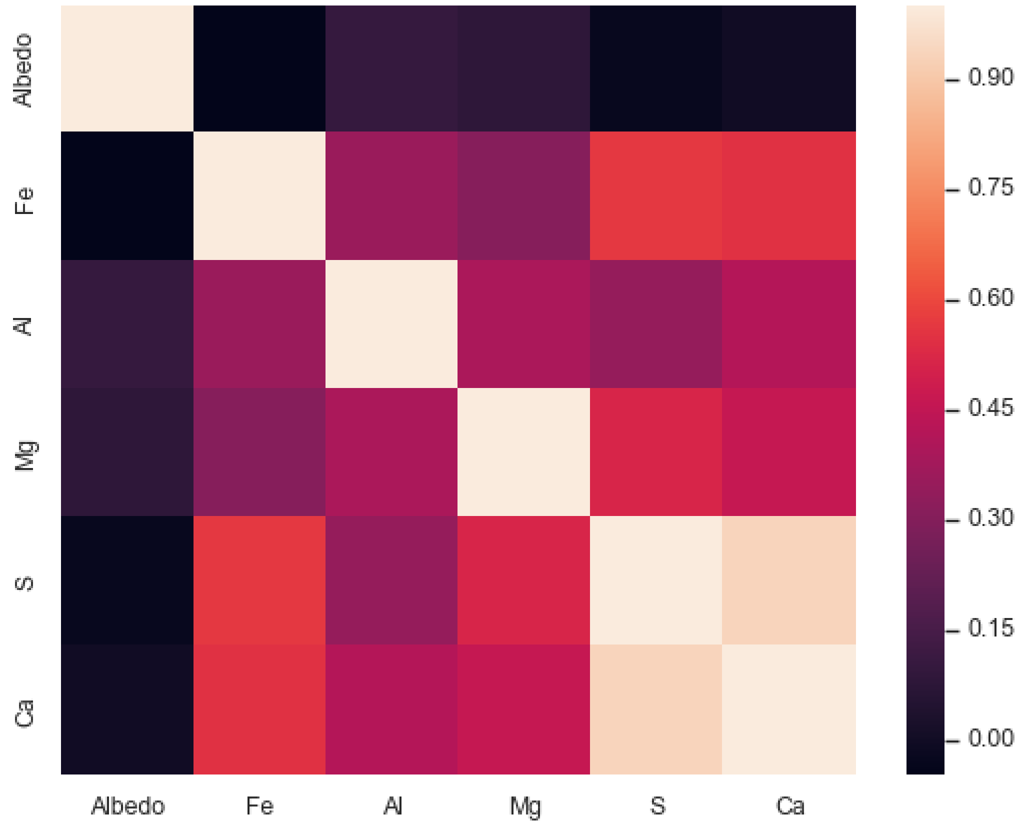
	Albedo	Fe	Al	Mg	S	Ca
Albedo	1.000000	-0.045356	0.101683	0.084904	-0.024850	0.002648
Fe	-0.045356	1.000000	0.355446	0.307113	0.565331	0.549103
Al	0.101683	0.355446	1.000000	0.399451	0.344053	0.417360
Mg	0.084904	0.307113	0.399451	1.000000	0.515704	0.462453
S	-0.024850	0.565331	0.344053	0.515704	1.000000	0.935043
Ca	0.002648	0.549103	0.417360	0.462453	0.935043	1.000000

In [25]:

```
sns.heatmap(train.corr())
```

Out[25]:

<matplotlib.axes._subplots.AxesSubplot at 0x2826deb8e08>

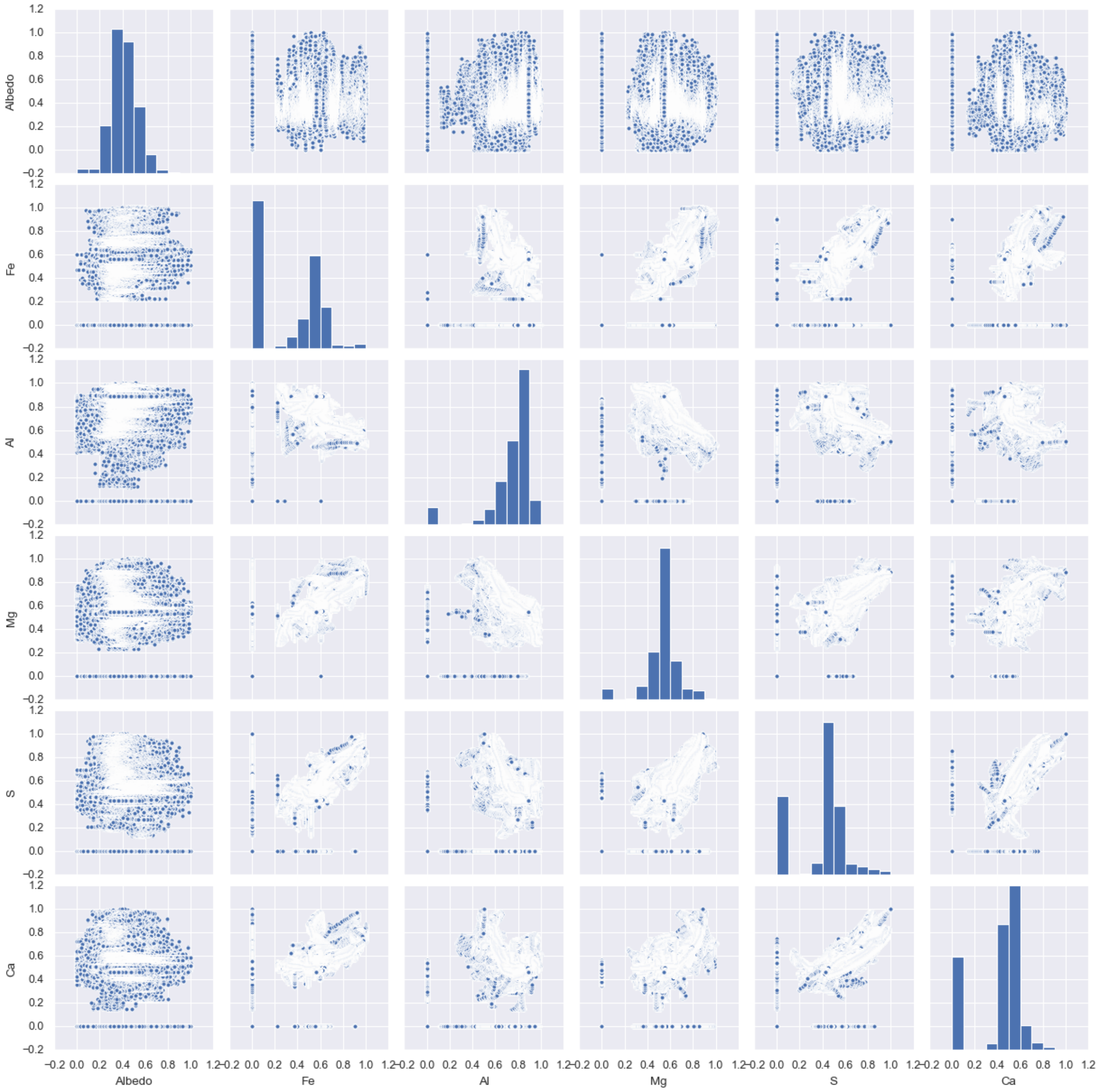


In [26]:

```
sns.pairplot(train)
```

Out[26]:

```
<seaborn.axisgrid.PairGrid at 0x2827938d888>
```



Ingsights from the plots above

1) Some of the variables are heavly skewed.

2) Little correlation can be obeserved among the dependent variables(which may not be useful for some of the models), and negligible correlation between albedo and chemical composition can be seen.

3) Due to the reasons mentioned above we cant expect very accurate and robust model

Multi Output Regression

In multioutput regression, typically the outputs are dependent upon the input and upon each other. This means that often the outputs are not independent of each other and may require a model that predicts both outputs together or each output contingent upon the other outputs.

Some regression machine learning algorithms support multiple outputs directly.

This includes most of the popular machine learning algorithms implemented in the scikit-learn library, such as:

LinearRegression KNeighborsRegressor RandomForestRegressor I will try the above models and I will also use the wrapper models such as Direct Multioutput Regression and Chained Multioutput Regression to check if XGboost, which gave good results previously, works well or not. At last I will use a more intuitive neural network model with 5 outputs and then use the bes model to predict for lower half of mercury albedo

For all the models these two steps will be followed :-

1) Fitting the regressor object on the hyperparameters obtained using GridSearch

2) Print the details about the evaluation metrics

Note the final peformace would be compared using Mean Square Error(MSE) as its a good evaluation metric for regression model

In [23]:

```
X = train.iloc[:, 0:1].values
y = train.iloc[:, 1:].values


from sklearn.preprocessing import StandardScaler

sc_X = StandardScaler()
sc_y = StandardScaler()
X_train = sc_X.fit_transform(X.reshape(X.shape[0],1))
y_train =  sc_y.fit_transform(y)
```

In [60]:

```
#Linear Regression

from sklearn.linear_model import LinearRegression
regressor = LinearRegression()
regressor.fit(X_train, y_train)

y_pred = regressor.predict(X_train)

print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
MAE: 0.16969612770922382
MSE: 0.0493852192423984
RMSE: 0.22222785433513595
```

KNN

In [61]:

```
!pip install KNeighboursRegressor
from sklearn.neighbors import KNeighborsRegressor
error_rate=[]
for i in range(1,30,2):

    knn = KNeighborsRegressor(n_neighbors=i,metric='euclidean')
    knn.fit(X_train,y_train)
    pred_i = knn.predict(X_train)
    print('k=>',i,' error',metrics.mean_squared_error(pred_i,y_train))
    error_rate.append(metrics.mean_squared_error(pred_i,y_train))
```

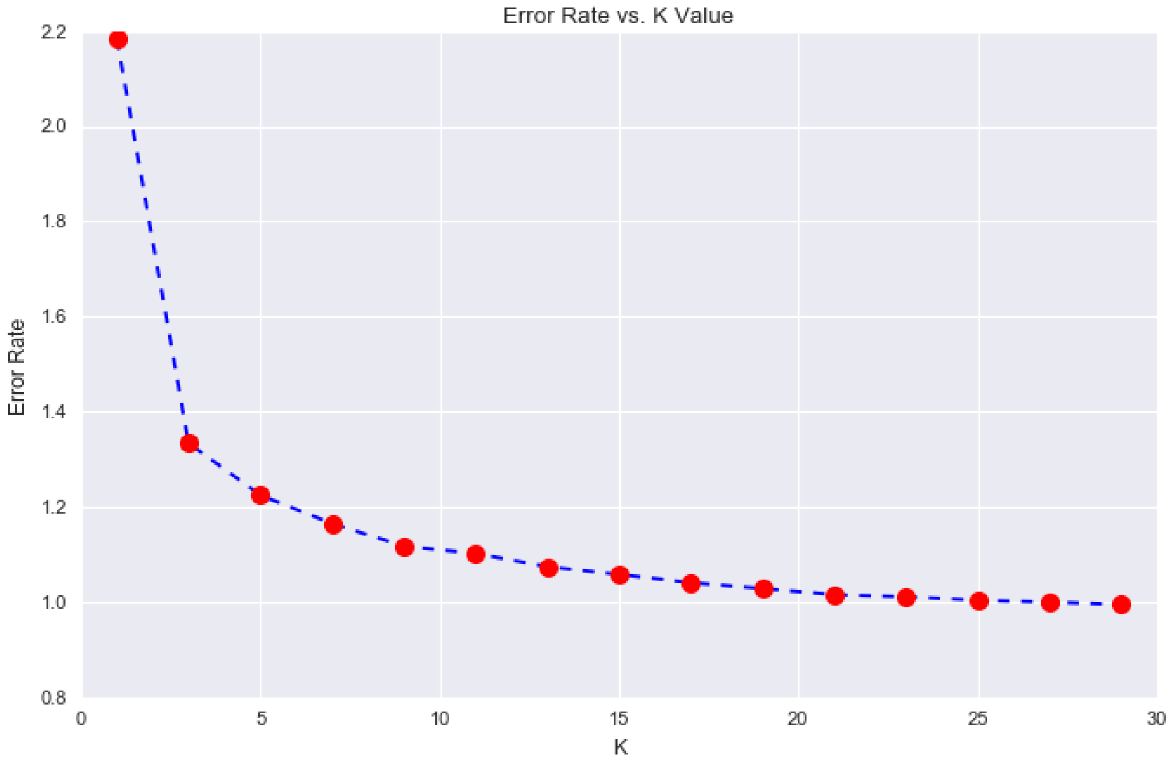
```
ERROR: Could not find a version that satisfies the requirement KNeighboursRe
gressor (from versions: none)
ERROR: No matching distribution found for KNeighboursRegressor

k=> 1  error 2.184374232946872
k=> 3  error 1.333497379138232
k=> 5  error 1.224230410936036
k=> 7  error 1.1642886779298178
k=> 9  error 1.116970379850421
k=> 11  error 1.1013871995249311
k=> 13  error 1.0739739978444232
k=> 15  error 1.0572072373202726
k=> 17  error 1.0401268512487176
k=> 19  error 1.0277888185211488
k=> 21  error 1.015049759955945
k=> 23  error 1.010429942571362
k=> 25  error 1.0031161787506917
k=> 27  error 0.9991183228647094
k=> 29  error 0.9940815288833476
```

In [62]:

```
plt.figure(figsize=(10,6))
plt.plot(range(1,30,2),error_rate,color='blue', linestyle='dashed', marker='o',
         markerfacecolor='red', markersize=10)
plt.title('Error Rate vs. K Value')
plt.xlabel('K')
plt.ylabel('Error Rate')
```

Out[62]:

```
Text(0, 0.5, 'Error Rate')
```



In [63]:

```
regressor.fit(X_train, y_train)
y_pred = regressor.predict(X_train)

print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
MAE: 0.16969612770922382
MSE: 0.0493852192423984
RMSE: 0.22222785433513595
```

In [69]:

```
#Random Forest

from sklearn.model_selection import GridSearchCV
from sklearn.ensemble import RandomForestRegressor

param_grid = [
{'n_estimators': [100,100,100],
 'max_depth': [5,10],
 'max_features' : ['auto', 'sqrt', 'log2'],
'min_samples_leaf':[5,10]


}
]

grid_search_forest = GridSearchCV(regressor, param_grid, cv=2,verbose=5)
grid_search_forest.fit(X_train, y_train)

grid_search_forest.best_params_
```

```
Fitting 2 folds for each of 36 candidates, totalling 72 fits
[CV] max_depth=5, max_features=auto, min_samples_leaf=5, n_estimators=100

[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent work
ers.

---------------------------------------------------------------------------
-
ValueError                                Traceback (most recent call las
t)
<ipython-input-69-bde9d60debdb> in <module>
     15 
     16 grid_search_forest = GridSearchCV(regressor, param_grid, cv=2,verb
ose=5)
---> 17 grid_search_forest.fit(X_train, y_train)
     18 
     19 grid_search_forest.best_params_

E:\anxe\lib\site-packages\sklearn\model_selection\_search.py in fit(self,
 X, y, groups, **fit_params)
    708                 return results
    709 
--> 710             self._run_search(evaluate_candidates)
    711 
    712         # For multi-metric evaluation, store the best_index_, best
_params_ and

E:\anxe\lib\site-packages\sklearn\model_selection\_search.py in _run_searc
h(self, evaluate_candidates)
   1149     def _run_search(self, evaluate_candidates):
   1150         """Search all candidates in param_grid"""
-> 1151         evaluate_candidates(ParameterGrid(self.param_grid))
   1152 
   1153 

E:\anxe\lib\site-packages\sklearn\model_selection\_search.py in evaluate_c
andidates(candidate_params)
    687                                for parameters, (train, test)
    688                                in product(candidate_params,
```

```
--> 689                                        cv.split(X, y, groups)))
    690 
    691                 if len(out) < 1:

E:\anxe\lib\site-packages\joblib\parallel.py in __call__(self, iterable)
   1002             # remaining jobs.
   1003             self._iterating = False
-> 1004             if self.dispatch_one_batch(iterator):
   1005                 self._iterating = self._original_iterator is not N
one
   1006 

E:\anxe\lib\site-packages\joblib\parallel.py in dispatch_one_batch(self, i
terator)
    833                 return False
    834             else:
--> 835                 self._dispatch(tasks)
    836                 return True
    837 

E:\anxe\lib\site-packages\joblib\parallel.py in _dispatch(self, batch)
    752         with self._lock:
    753             job_idx = len(self._jobs)
--> 754             job = self._backend.apply_async(batch, callback=cb)
    755             # A job can complete so quickly than its callback is
    756             # called before we get here, causing self._jobs to

E:\anxe\lib\site-packages\joblib\_parallel_backends.py in apply_async(sel
f, func, callback)
    207     def apply_async(self, func, callback=None):
    208         """Schedule a func to be run"""
--> 209         result = ImmediateResult(func)
    210         if callback:
    211             callback(result)

E:\anxe\lib\site-packages\joblib\_parallel_backends.py in __init__(self, b
atch)
    588         # Don't delay the application, to avoid keeping the input
    589         # arguments in memory
--> 590         self.results = batch()
    591 
    592     def get(self):

E:\anxe\lib\site-packages\joblib\parallel.py in __call__(self)
    254         with parallel_backend(self._backend, n_jobs=self._n_jobs):
    255             return [func(*args, **kwargs)
--> 256                     for func, args, kwargs in self.items]
    257 
    258     def __len__(self):

E:\anxe\lib\site-packages\joblib\parallel.py in <listcomp>(.0)
    254         with parallel_backend(self._backend, n_jobs=self._n_jobs):
    255             return [func(*args, **kwargs)
--> 256                     for func, args, kwargs in self.items]
    257 
    258     def __len__(self):

E:\anxe\lib\site-packages\sklearn\model_selection\_validation.py in _fit_a
nd_score(estimator, X, y, scorer, train, test, verbose, parameters, fit_pa
rams, return_train_score, return_parameters, return_n_test_samples, return
_times, return_estimator, error_score)
```

```
    502                 cloned_parameters[k] = clone(v, safe=False)
    503
--> 504             estimator = estimator.set_params(**cloned_parameters)
    505
    506         start_time = time.time()

E:\anxe\lib\site-packages\sklearn\base.py in set_params(self, **params)
    234                                      'Check the list of available para
meters '
    235                                      'with `estimator.get_params().key
s()`.' %
--> 236                                      (key, self))
    237
    238                 if delim:

ValueError: Invalid parameter max_depth for estimator LinearRegression(cop
y_X=True, fit_intercept=True, n_jobs=None, normalize=False). Check the lis
t of available parameters with `estimator.get_params().keys()`.
```

In [48]:

```
from sklearn.ensemble import RandomForestRegressor
rf = RandomForestRegressor(max_depth=10,min_samples_leaf=5,n_estimators=10)
error_rate_train=[]

for iter in range(10):
    rf.fit(X_train, y_train)
    y_train_predicted = rf.predict(X_train)
    mse_train = metrics.mean_squared_error(y_train, y_train_predicted)
    error_rate_train.append( metrics.mean_squared_error(y_train, y_train_predicted))
    print("n_estimators: {} Train mse: {} ".format(rf.n_estimators , mse_train))
    rf.n_estimators += 100

error_rate_train
```

```
n_estimators: 10 Train mse: 0.07977552030294054
n_estimators: 110 Train mse: 0.07977437796606113
n_estimators: 210 Train mse: 0.07977406477018181
n_estimators: 310 Train mse: 0.07977403791126961
n_estimators: 410 Train mse: 0.07977410965649483
n_estimators: 510 Train mse: 0.07977399013465093
n_estimators: 610 Train mse: 0.07977406731641595
n_estimators: 710 Train mse: 0.07977407981554832
n_estimators: 810 Train mse: 0.07977404970563212
n_estimators: 910 Train mse: 0.07977407938691256
```

Out[48]:

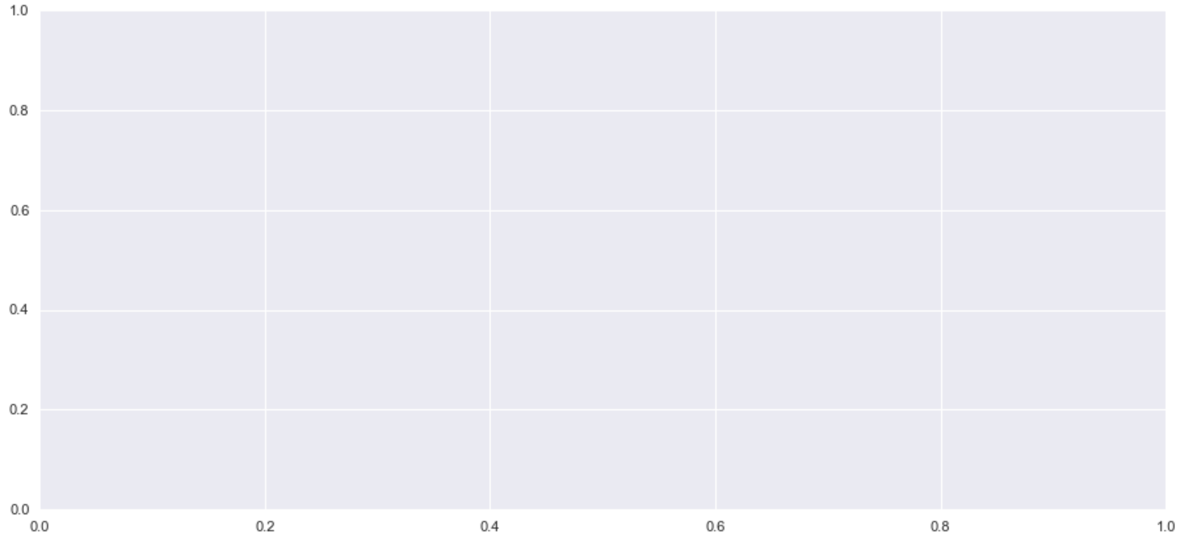
```
[0.07977552030294054,
 0.07977437796606113,
 0.07977406477018181,
 0.07977403791126961,
 0.07977410965649483,
 0.07977399013465093,
 0.07977406731641595,
 0.07977407981554832,
 0.07977404970563212,
 0.07977407938691256]
```

In [54]:

```
plt.figure(figsize=(14,6))


plt.style.use('seaborn')
plt.plot(range(10,610,100),error_rate_train, label = 'Training error')
#plt.plot(range(100,1200,100),error_rate_test, label = 'Validation error')
plt.ylabel('MSE', fontsize = 14)
plt.xlabel('N_estimators', fontsize = 14)
plt.legend()
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-54-f6e5abd33261> in <module>
      3 
      4 plt.style.use('seaborn')
----> 5 plt.plot(range(10,610,100),error_rate_train, label = 'Training error')
      6 #plt.plot(range(100,1200,100),error_rate_test, label = 'Validation error')
      7 plt.ylabel('MSE', fontsize = 14)

E:\anxe\lib\site-packages\matplotlib\pyplot.py in plot(scalex, scaley, data, *args, **kwargs)
   2794     return gca().plot(
   2795         *args, scalex=scalex, scaley=scaley, **({"data": data} if data
-> 2796         is not None else {}), **kwargs)
   2797 
   2798 

E:\anxe\lib\site-packages\matplotlib\axes\_axes.py in plot(self, scalex, scaley, data, *args, **kwargs)
   1663         """
   1664         kwargs = cbook.normalize_kwargs(kwargs, mlines.Line2D._alias_map)
-> 1665         lines = [*self._get_lines(*args, data=data, **kwargs)]
   1666         for line in lines:
   1667             self.add_line(line)

E:\anxe\lib\site-packages\matplotlib\axes\_base.py in __call__(self, *args, **kwargs)
    223                 this += args[0],
    224                 args = args[1:]
--> 225             yield from self._plot_args(this, kwargs)
    226 
    227     def get_next_color(self):

E:\anxe\lib\site-packages\matplotlib\axes\_base.py in _plot_args(self, tup, kwargs)
    389             x, y = index_of(tup[-1])
    390 
--> 391         x, y = self._xy_from_xy(x, y)
    392 
    393         if self.command == 'plot':

E:\anxe\lib\site-packages\matplotlib\axes\_base.py in _xy_from_xy(self, x,
```

```
y)
    268         if x.shape[0] != y.shape[0]:
    269             raise ValueError("x and y must have same first dimensi
on, but "
--> 270                              "have shapes {} and {}".format(x.shap
e, y.shape))
    271         if x.ndim > 2 or y.ndim > 2:
    272             raise ValueError("x and y can be no greater than 2-D,
 but have "

ValueError: x and y must have same first dimension, but have shapes (6,) a
nd (10,)
```



In [59]:

```
regressor = RandomForestRegressor(max_depth=10,min_samples_leaf=5,n_estimators=210)

# fit the regressor with x and y data
regressor.fit(X_train, y_train)
y_pred = regressor.predict(X_train)

print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
MAE: 0.16040761617236346
MSE: 0.0460496631614707
RMSE: 0.21459185250486726
```

Xgboost using MultiOutputRegressor wrapper

How normal MultiOutputRegressor works :-

For example, if a multioutput regression problem required the prediction of three values y1, y2 and y3 given an input X, then this could be partitioned into three single-output regression problems:

Problem 1: Given X, predict y1.

Problem 2: Given X, predict y2.

Problem 3: Given X, predict y3.

In [58]:

```
from sklearn.multioutput import MultiOutputRegressor
regressor=xgboost.XGBRegressor()


wrapper = MultiOutputRegressor(regressor)
wrapper.fit(X_train,y_train)
y_pred = wrapper.predict(X_train)

print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
MAE: 0.16040049621548919
MSE: 0.04604761323853671
RMSE: 0.2145870761218781
```

In [38]:

```
import pickle
filename = 'Best_Model_XG_boost.sav'
pickle.dump(regressor, open(filename, 'wb'))
```

Xgboost using Chained Multioutput Regression wrapper

How normal Chained MultiOutputRegressor works :-

For example, if a multioutput regression problem required the prediction of three values y1, y2 and y3 given an input X, then this could be partitioned into three dependent single-output regression problems as follows:

Problem 1: Given X, predict y1.

Problem 2: Given X and yhat1, predict y2.

Problem 3: Given X, yhat1, and yhat2, predict y3.

In [57]:

```
from sklearn.multioutput import RegressorChain
!conda install -c conda-forge xgboost
import xgboost
regressor=xgboost.XGBRegressor()

wrapper =RegressorChain(regressor)
wrapper.fit(X_train,y_train)
y_pred = wrapper.predict(X_train)

print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
Collecting package metadata (current_repodata.json): ...working... done
Solving environment: ...working... done

# All requested packages already installed.

MAE: 0.16274678386662955
MSE: 0.05224619983675919
RMSE: 0.228574276410884
```

Neural Network

In [40]:

```
!pip install tensorflow
import tensorflow as tf
from tensorflow.keras.layers import Input, Dense, Activation,Dropout
from tensorflow.keras.models import Model
from tensorflow import keras
```

```
Requirement already satisfied: tensorflow in e:\anxe\lib\site-packages (2.4.
1)
Requirement already satisfied: opt-einsum~=3.3.0 in e:\anxe\lib\site-package
s (from tensorflow) (3.3.0)
Requirement already satisfied: google-pasta~=0.2 in e:\anxe\lib\site-package
s (from tensorflow) (0.2.0)
Requirement already satisfied: numpy~=1.19.2 in e:\anxe\lib\site-packages (f
rom tensorflow) (1.19.5)
Requirement already satisfied: six~=1.15.0 in e:\anxe\lib\site-packages (fro
m tensorflow) (1.15.0)
Requirement already satisfied: keras-preprocessing~=1.1.2 in e:\anxe\lib\sit
e-packages (from tensorflow) (1.1.2)
Requirement already satisfied: tensorboard~=2.4 in e:\anxe\lib\site-packages
(from tensorflow) (2.4.1)
Requirement already satisfied: flatbuffers~=1.12.0 in e:\anxe\lib\site-packa
ges (from tensorflow) (1.12)
Requirement already satisfied: absl-py~=0.10 in e:\anxe\lib\site-packages (f
rom tensorflow) (0.12.0)
Requirement already satisfied: typing-extensions~=3.7.4 in e:\anxe\lib\site-
packages (from tensorflow) (3.7.4.3)
Requirement already satisfied: grpcio~=1.32.0 in e:\anxe\lib\site-packages
(from tensorflow) (1.32.0)
Requirement already satisfied: wrapt~=1.12.1 in e:\anxe\lib\site-packages (f
rom tensorflow) (1.12.1)
Requirement already satisfied: termcolor~=1.1.0 in e:\anxe\lib\site-packages
(from tensorflow) (1.1.0)
Requirement already satisfied: gast==0.3.3 in e:\anxe\lib\site-packages (fro
m tensorflow) (0.3.3)
Requirement already satisfied: protobuf>=3.9.2 in e:\anxe\lib\site-packages
(from tensorflow) (3.15.8)
Requirement already satisfied: tensorflow-estimator<2.5.0,>=2.4.0 in e:\anxe
\lib\site-packages (from tensorflow) (2.4.0)
Requirement already satisfied: wheel~=0.35 in e:\anxe\lib\site-packages (fro
m tensorflow) (0.36.2)
Requirement already satisfied: astunparse~=1.6.3 in e:\anxe\lib\site-package
s (from tensorflow) (1.6.3)
Requirement already satisfied: h5py~=2.10.0 in e:\anxe\lib\site-packages (fr
om tensorflow) (2.10.0)
Requirement already satisfied: google-auth-oauthlib<0.5,>=0.4.1 in e:\anxe\l
ib\site-packages (from tensorboard~=2.4->tensorflow) (0.4.4)
Requirement already satisfied: markdown>=2.6.8 in e:\anxe\lib\site-packages
(from tensorboard~=2.4->tensorflow) (3.3.4)
Requirement already satisfied: google-auth<2,>=1.6.3 in e:\anxe\lib\site-pac
kages (from tensorboard~=2.4->tensorflow) (1.28.1)
Requirement already satisfied: tensorboard-plugin-wit>=1.6.0 in e:\anxe\lib
\site-packages (from tensorboard~=2.4->tensorflow) (1.8.0)
Requirement already satisfied: requests<3,>=2.21.0 in e:\anxe\lib\site-packa
ges (from tensorboard~=2.4->tensorflow) (2.22.0)
Requirement already satisfied: werkzeug>=0.11.15 in e:\anxe\lib\site-package
s (from tensorboard~=2.4->tensorflow) (1.0.0)
Requirement already satisfied: setuptools>=41.0.0 in e:\anxe\lib\site-packag
es (from tensorboard~=2.4->tensorflow) (45.2.0.post20200210)
Requirement already satisfied: requests-oauthlib>=0.7.0 in e:\anxe\lib\site-
```

```
packages (from google-auth-oauthlib<0.5,>=0.4.1->tensorboard~=2.4->tensorflo
w) (1.3.0)
Requirement already satisfied: importlib-metadata; python_version < "3.8" in
e:\anxe\lib\site-packages (from markdown>=2.6.8->tensorboard~=2.4->tensorflo
w) (1.5.0)
Requirement already satisfied: cachetools<5.0,>=2.0.0 in e:\anxe\lib\site-pa
ckages (from google-auth<2,>=1.6.3->tensorboard~=2.4->tensorflow) (4.2.1)
Requirement already satisfied: rsa<5,>=3.1.4; python_version >= "3.6" in
e:\anxe\lib\site-packages (from google-auth<2,>=1.6.3->tensorboard~=2.4->ten
sorflow) (4.7.2)
Requirement already satisfied: pyasn1-modules>=0.2.1 in e:\anxe\lib\site-pac
kages (from google-auth<2,>=1.6.3->tensorboard~=2.4->tensorflow) (0.2.8)
Requirement already satisfied: certifi>=2017.4.17 in e:\anxe\lib\site-packag
es (from requests<3,>=2.21.0->tensorboard~=2.4->tensorflow) (2019.11.28)
Requirement already satisfied: idna<2.9,>=2.5 in e:\anxe\lib\site-packages
(from requests<3,>=2.21.0->tensorboard~=2.4->tensorflow) (2.8)
Requirement already satisfied: chardet<3.1.0,>=3.0.2 in e:\anxe\lib\site-pac
kages (from requests<3,>=2.21.0->tensorboard~=2.4->tensorflow) (3.0.4)
Requirement already satisfied: urllib3!=1.25.0,!=1.25.1,<1.26,>=1.21.1 in
e:\anxe\lib\site-packages (from requests<3,>=2.21.0->tensorboard~=2.4->tenso
rflow) (1.25.8)
Requirement already satisfied: oauthlib>=3.0.0 in e:\anxe\lib\site-packages
(from requests-oauthlib>=0.7.0->google-auth-oauthlib<0.5,>=0.4.1->tensorboar
d~=2.4->tensorflow) (3.1.0)
Requirement already satisfied: zipp>=0.5 in e:\anxe\lib\site-packages (from
importlib-metadata; python_version < "3.8"->markdown>=2.6.8->tensorboard~=2.
4->tensorflow) (2.2.0)
Requirement already satisfied: pyasn1>=0.1.3 in e:\anxe\lib\site-packages (f
rom rsa<5,>=3.1.4; python_version >= "3.6"->google-auth<2,>=1.6.3->tensorboa
rd~=2.4->tensorflow) (0.4.8)
```

In [41]:

```python
def create_model(learn_rate=0.01):
    model = tf.keras.Sequential()
    model.add(tf.keras.layers.Dense(2))
    model.add(tf.keras.layers.Dense(10))
    model.add(tf.keras.layers.Dense(5))

    opt = keras.optimizers.Adam(learning_rate=learn_rate)
    model.compile(loss='mse', optimizer=opt)
    return model
```

In [43]:

```
from sklearn.model_selection import GridSearchCV
from keras.wrappers.scikit_learn import KerasRegressor

model = KerasRegressor(build_fn=create_model,verbose=4)
learn_rate = [0.001,0.01,0.1,1]
batch_size = [32]
epochs = [10]
param_grid = dict(learn_rate=learn_rate,batch_size=batch_size,epochs=epochs)

grid = GridSearchCV(estimator=model, param_grid=param_grid, cv=2,verbose=10)
grid_result = grid.fit(X_train, y_train)
```

```
Fitting 2 folds for each of 4 candidates, totalling 8 fits
[CV] batch_size=32, epochs=10, learn_rate=0.001 ......................

[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent wo
rkers.

Epoch 1/10
Epoch 2/10
Epoch 3/10
Epoch 4/10
Epoch 5/10
Epoch 6/10
Epoch 7/10
Epoch 8/10
Epoch 9/10
Epoch 10/10
[CV]  batch_size=32, epochs=10, learn_rate=0.001, score=-2.213, total= 1.3
min
[CV] batch_size=32, epochs=10, learn_rate=0.001 ......................
Epoch 1/10
```

In [45]:

```
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
```

```
Best: -1.574849 using {'batch_size': 32, 'epochs': 10, 'learn_rate': 0.01}
```

In [46]:

```
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(2))
model.add(tf.keras.layers.Dense(10))
model.add(tf.keras.layers.Dense(5))
opt = keras.optimizers.Adam(learning_rate=0.001)

model.compile(optimizer='AdaGrad', loss='mse')
# This builds the model for the first time:
history  = model.fit(X_train, y_train, batch_size=32, epochs=10)
```

```
Epoch 1/10
32400/32400 [==============================] - 19s 573us/step - loss: 1.0005
Epoch 2/10
32400/32400 [==============================] - 18s 557us/step - loss: 0.9956
Epoch 3/10
32400/32400 [==============================] - 18s 552us/step - loss: 0.9954
Epoch 4/10
32400/32400 [==============================] - 19s 573us/step - loss: 0.9954
Epoch 5/10
32400/32400 [==============================] - 19s 573us/step - loss: 0.9943
Epoch 6/10
32400/32400 [==============================] - 18s 570us/step - loss: 0.9947
Epoch 7/10
32400/32400 [==============================] - 19s 575us/step - loss: 0.9955
Epoch 8/10
32400/32400 [==============================] - 19s 579us/step - loss: 0.9940
Epoch 9/10
32400/32400 [==============================] - 19s 575us/step - loss: 0.9955
Epoch 10/10
32400/32400 [==============================] - 19s 582us/step - loss: 0.9939
```

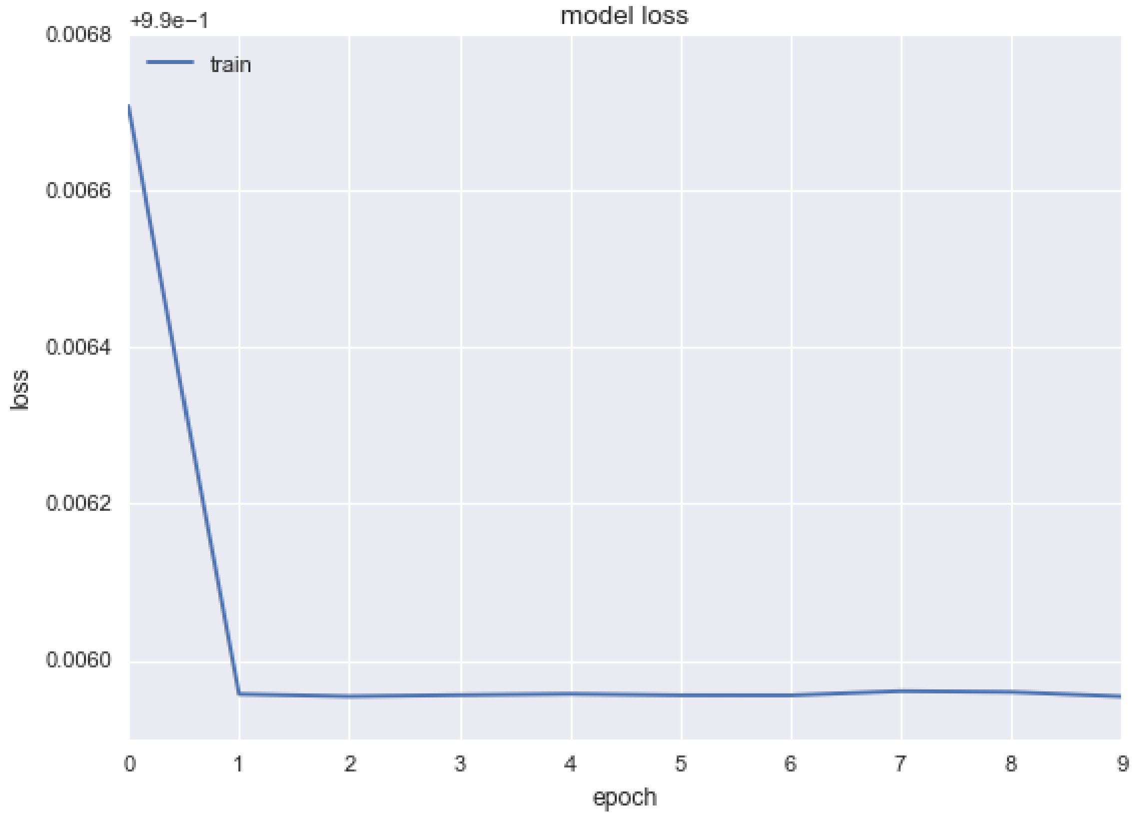
In [47]:

```
model.summary()
```

```
Model: "sequential_9"
_________________________________________________________________
Layer (type)                 Output Shape              Param #   
=================================================================
dense_27 (Dense)             (32, 2)                   4         
_________________________________________________________________
dense_28 (Dense)             (32, 10)                  30        
_________________________________________________________________
dense_29 (Dense)             (32, 5)                   55        
=================================================================
Total params: 89
Trainable params: 89
Non-trainable params: 0
_________________________________________________________________
```

In [48]:

```
plt.plot(history.history['loss'])
plt.title('model loss')
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['train', 'test'], loc='upper left')
plt.show()
```



In [54]:

```
import sklearn.metrics as metrics
y_pred = model.predict(X_train)

print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
MAE: 0.16969917412352442
MSE: 0.04938523022003832
RMSE: 0.2222278790341984
```

Sklearn's - Neural Network

Regressor(MLPRegressor)

In [50]:

```
from sklearn.neural_network import MLPRegressor
regressor = MLPRegressor().fit(X_train, y_train)
y_pred = regressor.predict(X_train)
```

In [51]:

```
import sklearn.metrics as metrics
print('MAE:', metrics.mean_absolute_error(sc_y.inverse_transform(y_train), sc_y.inverse_tra
print('MSE:', metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inverse_tran
print('RMSE:', np.sqrt(metrics.mean_squared_error(sc_y.inverse_transform(y_train), sc_y.inv
```

```
MAE: 0.16059327403737073
MSE: 0.0460977998711275
RMSE: 0.21470398196383667
```

Final Results

The lowest MSE obtained was with the tuned XGBOOST model

MSE = 0.007991978600932065

Predicting for bottom half using this model

In [52]:

```
from sklearn.multioutput import RegressorChain
import xgboost
regressor=xgboost.XGBRegressor()
wrapper =RegressorChain(regressor)
wrapper.fit(X_train,y_train)

bottom_albedo = mercury_bottom.flatten()

test_predictions  = wrapper.predict(bottom_albedo.reshape(1036800,1))
```

In [53]:

```
test_final  = pd.DataFrame(sc_y.inverse_transform(test_predictions), columns = ['Fe','Al','

test_final.head()
```

Out[53]:

	Fe	Al	Mg	S	Ca
0	0.311038	0.818740	0.499021	0.467187	0.505842
1	0.307719	0.821952	0.501490	0.471599	0.508550
2	0.299610	0.811316	0.480175	0.371925	0.463273
3	0.307719	0.821952	0.501490	0.471599	0.508550
4	0.311038	0.818740	0.499021	0.467187	0.505842

Insights

Again as Expected XGboost with Multioutput Regression wrapper peformed fairly well.

The results were not as good as compared to the MOON model

Very low relation between albedo and compostion may be a reason. Also, extenstive hyperparater tuning couldnt be done due to lack of time and computational power

In [ ]:

```

```