Decision Tree Classifier - Structure energy Correlations

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In this code, I explored possible correlations between initial configuration of water molecule on a solid surface and the system's final energetic stability. This code uses a dataset of 5000 configurations of water molecule on a photocatalytic surface. I generated the data using molecular dynamics simulations. The data is not published. However, it can be provided under request and with my advisor's permission.

How does the code work? Our goal is to define a classifier that can predict energy group of a molecule configuration on a slab surface. steps to this end:

1. **Initial data analysis** check the features and how they relate to our target (energy)
2. **configuration space computation** compute configurational space parameters
3. **Kmeans clustering** to find clusters of energy.
4. **Second data analysis** analyze the relation between configurational space and clusters of total energy.
5. **Decision Tree Classifier** Train and test a decision tree model.

In [1]:
```
import pandas as pd
import seaborn as sns
import numpy as np
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
from sklearn.datasets import fetch_mldata
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.multiclass import OneVsRestClassifier
from sklearn.metrics import precision_recall_curve, roc_curve
from sklearn.preprocessing import label_binarize

import matplotlib.pyplot as plt
```

Initial data analysis

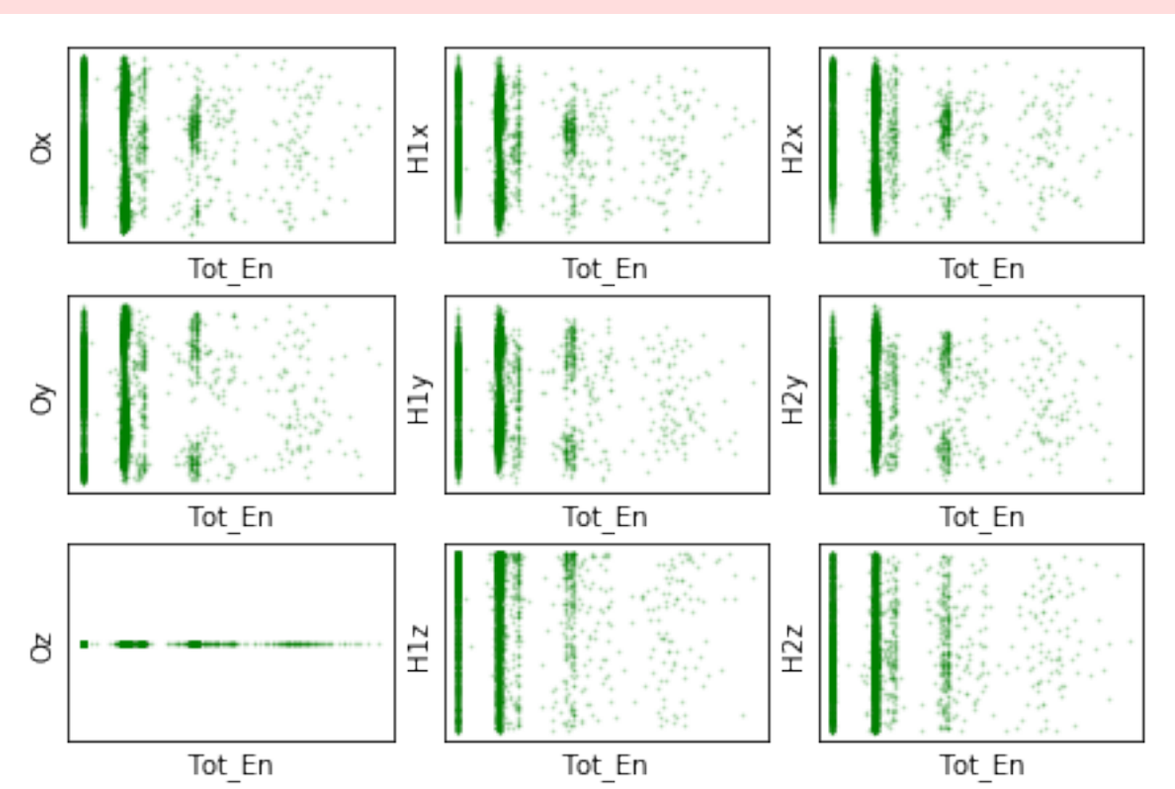
In [2]:
```
data = pd.read_csv("./water-init-pos-Ens.csv")
data.describe()
```

Out[2]:

	Ox	Oy	Oz	H1x	H1y	H1z	H2x	H2y	H2z	Tot_En
count	5000.000000	5000.000000	5.000000e+03	5000.000000	5000.000000	5000.000000	5000.000000	5000.000000	5000.000000	5000.000000
mean	10.520792	6.635305	1.791175e+01	10.518805	6.639893	18.235225	10.827397	6.582304	17.839640	-29755.696047
std	1.733909	1.747296	2.131841e-13	1.804560	1.817703	0.579350	1.824298	1.825966	0.509504	5.819200
min	7.282674	3.413599	1.791175e+01	6.575044	2.598014	16.941782	6.705610	2.624129	16.942175	-29760.600950
25%	8.994789	5.128800	1.791175e+01	9.017850	5.138938	17.787476	9.314482	5.062087	17.452681	-29760.595090
50%	10.529294	6.625549	1.791175e+01	10.517507	6.599615	18.409923	10.837341	6.570393	17.766267	-29754.822920
75%	12.023183	8.129761	1.791175e+01	12.017871	8.156384	18.759721	12.340088	8.089157	18.232416	-29754.472530
max	13.733497	9.917321	1.791175e+01	14.544109	10.778851	18.881750	14.611802	10.843835	18.880993	-29717.741840

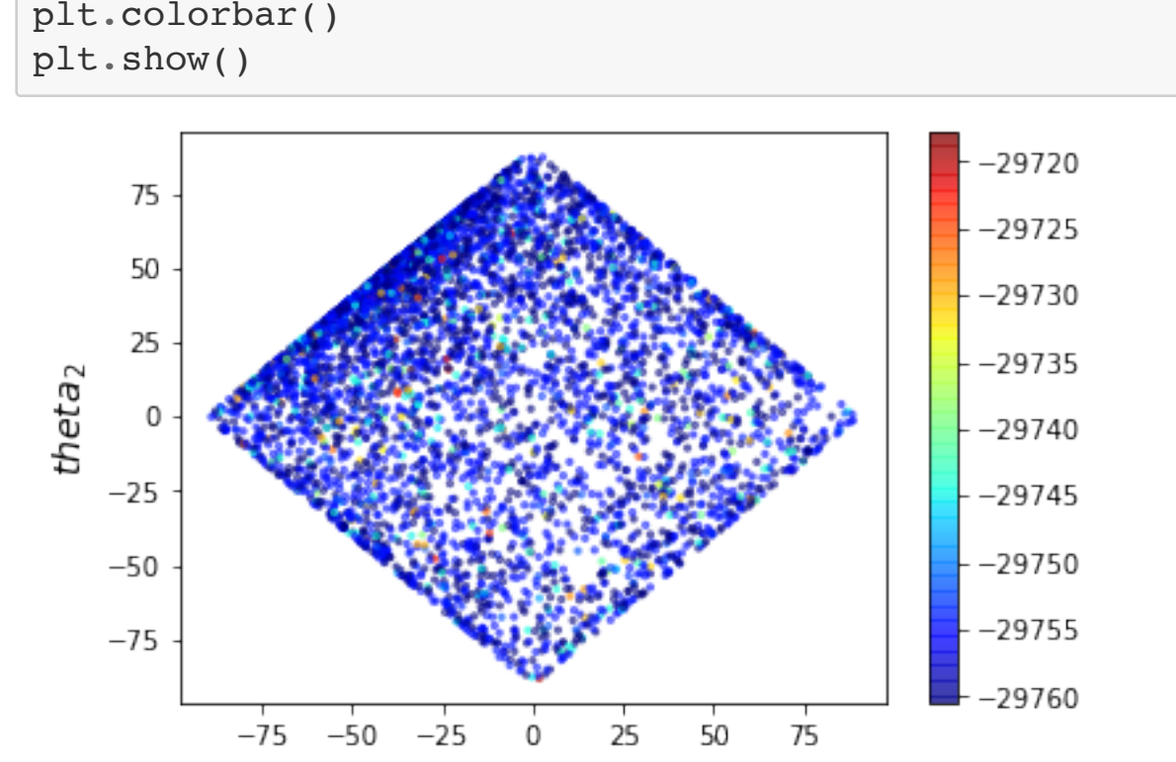
In [3]:
```
"""general data plot - x y z coordinate vs. total energy"""

nftoplot = 3
fig,axs = plt.subplots(nftoplot,nftoplot)
coords = ['Ox','Oy','Oz','H1x','H1y','H1z','H2x','H2y','H2z']

for i in range(nftoplot):
    for j in range(nftoplot):
        axs[i,j].plot(data['Tot_En'], data.iloc[:,i+3*j],'g.', alpha=.2, markersize=1.5)
        axs[i,j].set_xlabel('Tot_En')
        axs[i,j].set_ylabel(coords[i+3*j])
        axs[i,j].set_xticks([])
        axs[i,j].set_yticks([])

fig.tight_layout(pad=.5)
plt.show()
```

```
/Users/pmira002/.local/lib/python3.6/site-packages/matplotlib/cbook/__init__.py:1402: FutureWarning: Support for mult
i-dimensional indexing (e.g. `obj[:, None]`) is deprecated and will be removed in a future version.  Convert to a num
py array before indexing instead.
  x[:, None]
/Users/pmira002/.local/lib/python3.6/site-packages/matplotlib/axes/_base.py:276: FutureWarning: Support for multi-dim
ensional indexing (e.g. `obj[:, None]`) is deprecated and will be removed in a future version.  Convert to a numpy ar
ray before indexing instead.
  x = x[:, np.newaxis]
/Users/pmira002/.local/lib/python3.6/site-packages/matplotlib/axes/_base.py:278: FutureWarning: Support for multi-dim
ensional indexing (e.g. `obj[:, None]`) is deprecated and will be removed in a future version.  Convert to a numpy ar
ray before indexing instead.
  y = y[:, np.newaxis]
```

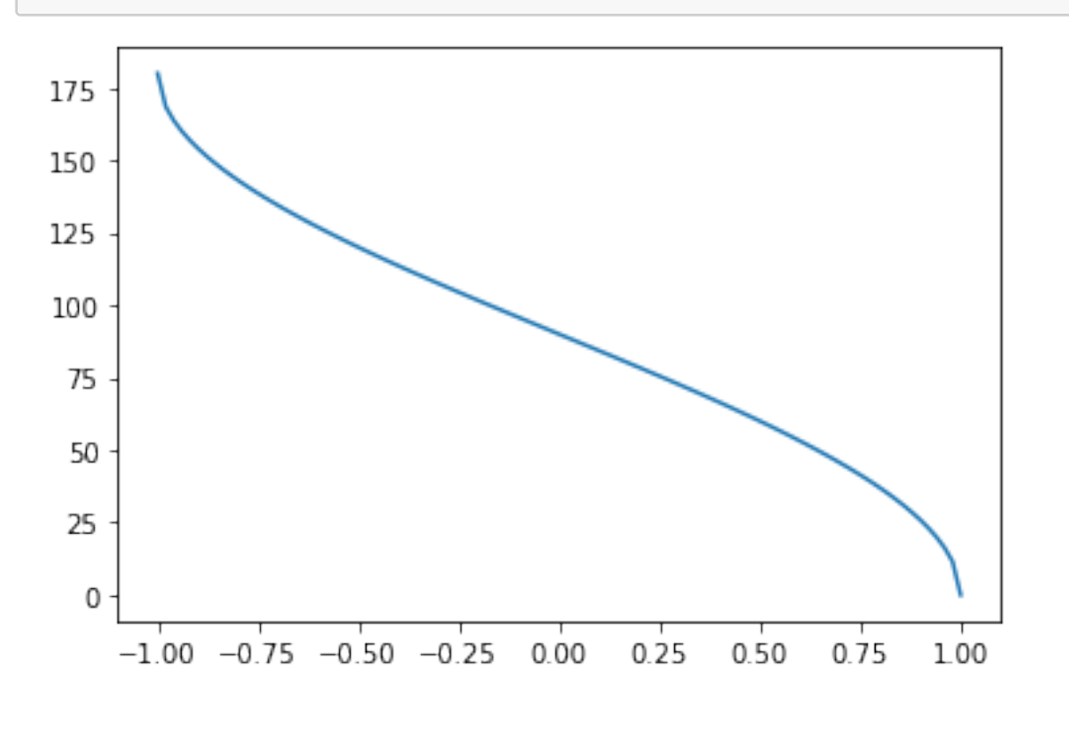


Configuration space computation

In [4]:
```
"""Compute configurational space:
   OH1 and OH2: matrices of shape (mx3) : OH bonds for all configurations in the dataset.
   n_bonds: matrix of shape (mx3) of normal vectors to the plane passing from OH1 and OH2.
   n_surf: matrix of shape (mx3) of normal vectors to the adsorbate surface plane.
   theta1: matrix of shape (mx3) of angle between n_surf and OH2 for all configurations.
   theta2: matrix of shape (mx3) of angle between n_surf and n_bonds for all configurations.
   plot theta1 vs. theta2 and color with energy value"""

O = data.iloc[:,:3].values
H1 = data.iloc[:,3:6].values
H2 = data.iloc[:,6:9].values
energy = data.Tot_En.values

OH1 = H1 - O
OH2 = H2 - O
V2 = OH1 + OH2
n_bonds = [np.cross(OH1[i],OH2[i]) for i in range(len(OH1))]
n_surf = [0,0,1]
m = len(data.values)

theta1 = []
theta2 = []
rad2degree = 180/np.pi

for j in range(m):
    v1 = n_bonds[j]
    v2 = V2[j]
    v3 = np.cross(v1,v2)
    dot1 = np.dot(n_surf,v2)

    norm1 = (np.linalg.norm(n_surf)*np.linalg.norm(v2))
    theta1.append((np.arccos(dot1/norm1))*rad2degree - 90)
    dot2 = np.dot(n_surf,v3)
    norm2 = (np.linalg.norm(n_surf)*np.linalg.norm(v3))
    theta2.append((np.arccos(dot2/norm2))*rad2degree - 90)



#plot
_ = plt.scatter(theta1, theta2, c=np.array(energy),cmap='jet', alpha=.5, s=5)
plt.xlabel(('$theta_1$'),fontsize=14)
plt.ylabel('$theta_2$',fontsize=14)
plt.colorbar()
plt.show()
```

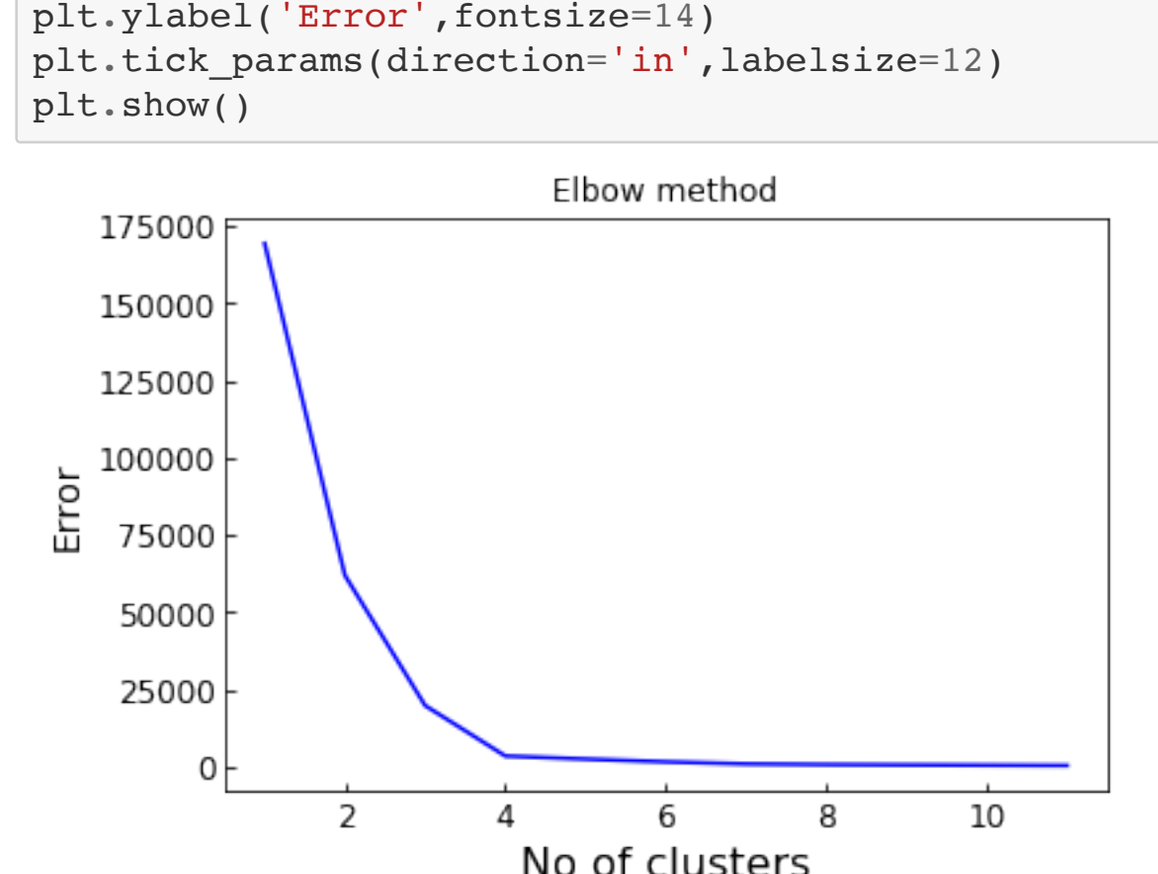


In [5]:
```
x = np.linspace(-1,1,100)
thx = np.arccos(x)*180/np.pi
plt.plot(x,thx)
plt.show()
```



Kmeans clustering

In [6]:
```
"""find k that minimizes error."""

y = energy[:,np.newaxis]

Err = []

for k in range(1,12):
    kmeans = KMeans(n_clusters=k, random_state=0)
    y_kmeans = kmeans.fit_predict(y)
    Err.append(kmeans.inertia_)

plt.plot(range(1,12),Err,'b')
plt.title('Elbow method',fontsize=12)
plt.xlabel('No of clusters',fontsize=16)
plt.ylabel('Error',fontsize=14)
plt.tick_params(direction='in',labelsize=12)
plt.show()
```

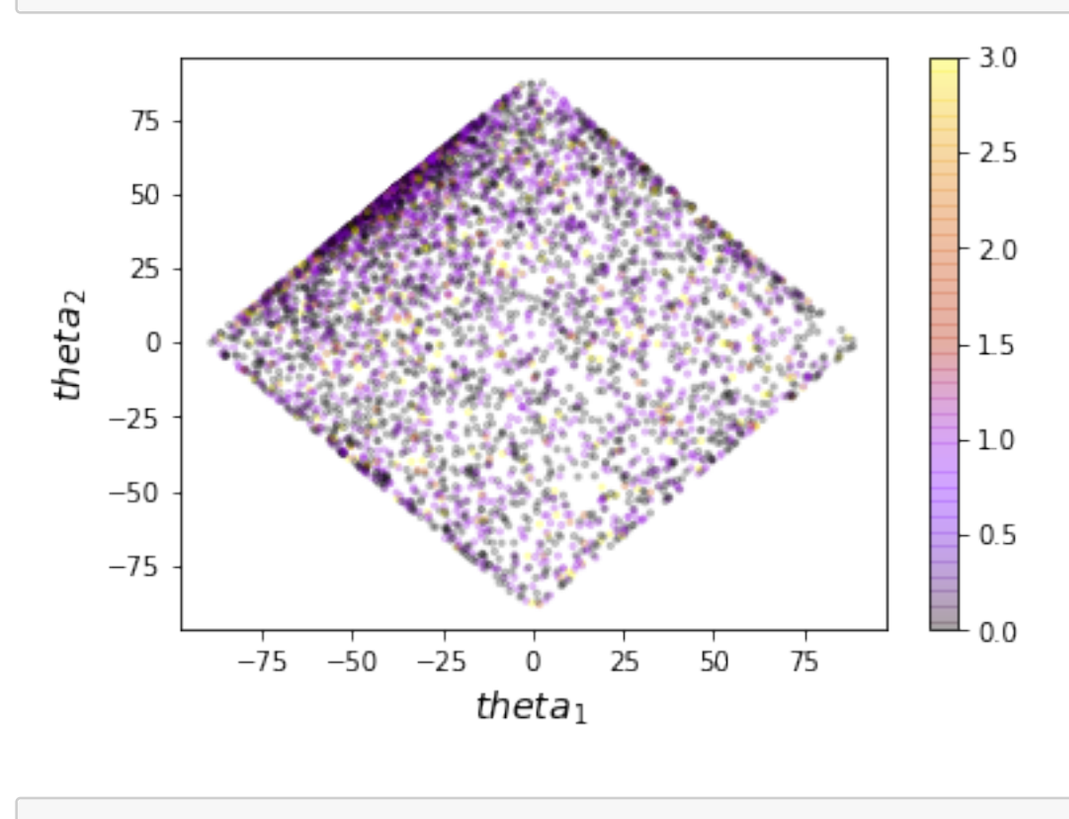


Cluster energies into 4 groups (k=4). Then plot angles again, but this time use clusters of energy for coloring.

In [7]:
```
kmeans4 = KMeans(n_clusters=4, random_state=0)
y_kmeans4 = kmeans4.fit_predict(y)
```

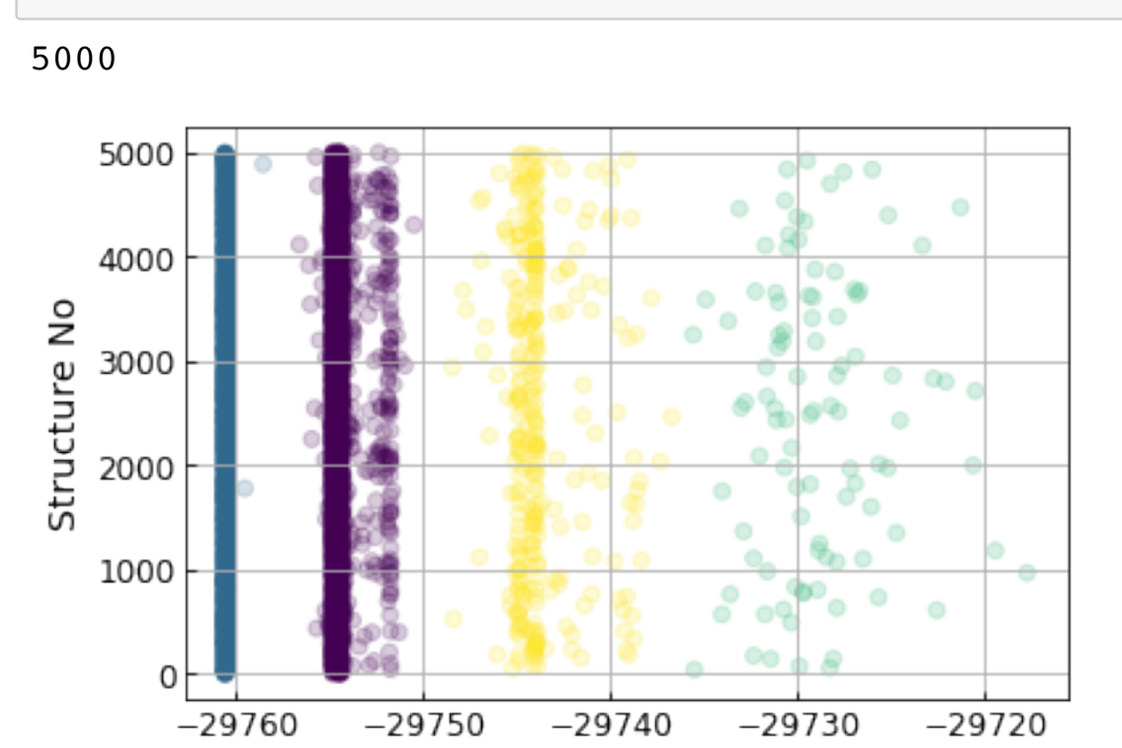
Second data analysis

In [8]:
```
_ = plt.scatter(theta1, theta2, c=y_kmeans4, cmap='gnuplot', alpha=.2, s=5)
plt.xlabel(('$theta_1$'),fontsize=14)
plt.ylabel('$theta_2$',fontsize=14)
plt.colorbar()
plt.show()
#plt.savefig('./angles-clustered-feats.png',dpi=200)
```

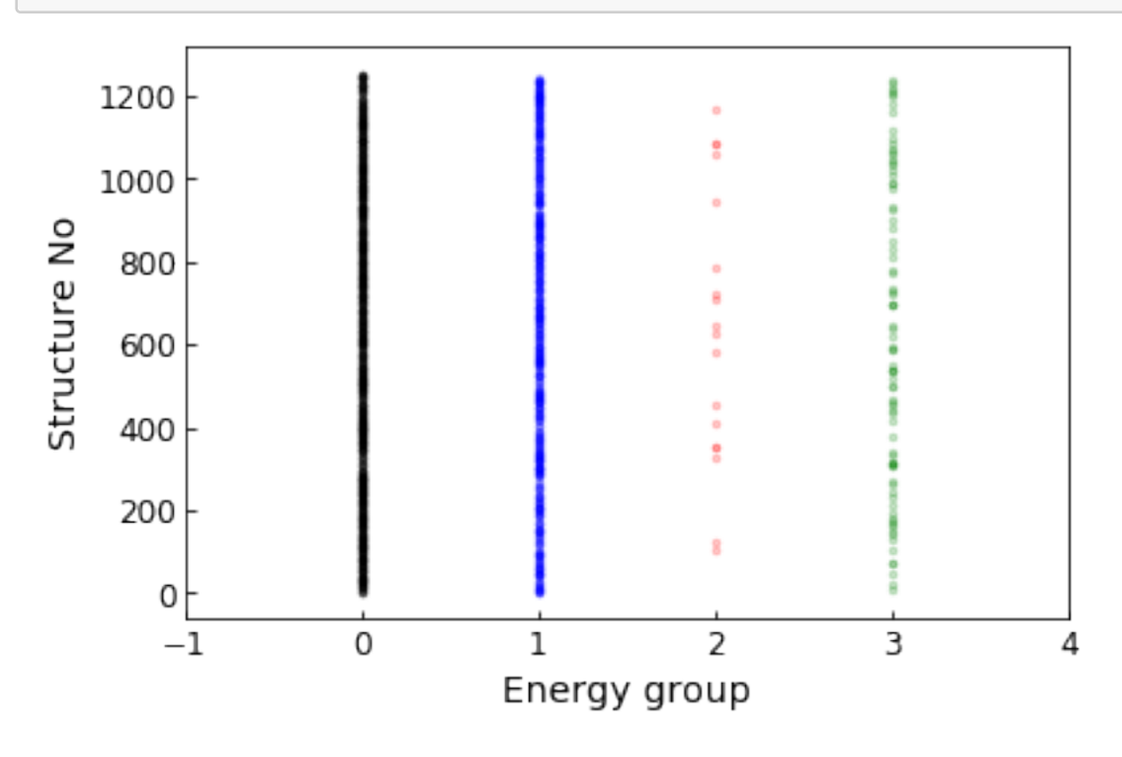


In [9]:
```
# plot of structural config. vs. final energetics
Configs = np.arange(1,5001)
print(Configs[-1])
cmap = ['r','b','g','m']

plt.scatter(data.Tot_En,Configs,c=y_kmeans4,alpha=.2)
plt.xlabel(('Total Energy ('r'$eV$)'),fontsize=14)
plt.ylabel('Structure No',fontsize=14)
plt.tick_params(direction='in',labelsize=12)
plt.grid(None)
plt.show()
```

```
5000
```



In [20]:
```
# plot of structural config. vs. group of final energetics
plt.figure()
plt.xlim(-1,np.max(y_kmeans4)+1)
Configs = np.arange(0,1250)
bounds = [-29757, -29749.5, -29736]

cmap = ['k','b','r','g']
for i,y in enumerate(y_kmeans4[3750:]):
    plt.scatter(y, Configs[i], c=cmap[y], s=6.5, alpha=.2)

plt.xlabel(('Energy group'),fontsize=14)
plt.ylabel('Structure No',fontsize=14)
plt.tick_params(direction='in',labelsize=12)
plt.show()
```



Decision Tree Classifier

In [15]:
```
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_absolute_error
from sklearn import tree


def MyTree(train_X,val_X,train_y,val_y,randomstate=1,max_leaf_nodes=100):

    #define model
    Water_on_ZnO = DecisionTreeClassifier(max_leaf_nodes=max_leaf_nodes, random_state=1)

    #fit the model on the Train set
    Water_on_ZnO.fit(train_X,train_y)

    #Predict output for the validation set
    ypred = Water_on_ZnO.predict(val_X)

    #validate model - check error
    MAE = mean_absolute_error (val_y, ypred)
    #print("mean_absolute_error is {}".format(MAE))

    avg_Val_y = (data.Tot_En[5000-int(5000*0.25):]).mean()

    Rel_MAE = MAE/avg_Val_y
    print("The ratio of MAE to the avg En value in the validation set is {}". format(abs(MAE/avg_Val_y)))

    y_score = Water_on_ZnO.predict_proba(val_X)

    return MAE, Rel_MAE,ypred, y_score


if __name__=='__main__':

    features = coords
    X = data[coords]
    X2 = np.vstack((theta1,theta2)).T
    print(np.shape(X2))
    print(np.shape(X))
    yc = y_kmeans4

    train_X, val_X, train_y, val_y = train_test_split(X, yc, test_size=0.25, random_state=0)
    MAE, Rel_MAE,ypred,y_score = MyTree(train_X,val_X,train_y,val_y)
    print("mean_absolute_error using coord. as features is {}".format(MAE))

    train_X2, val_X2, train_y2, val_y2 = train_test_split(X2, yc, test_size=0.25, random_state=0)
    MAE2, Rel_MAE2,ypred2,y_score2 = MyTree(train_X2,val_X2,train_y2,val_y2)
    print("mean_absolute_error using angles as features is {}".format(MAE2))
```

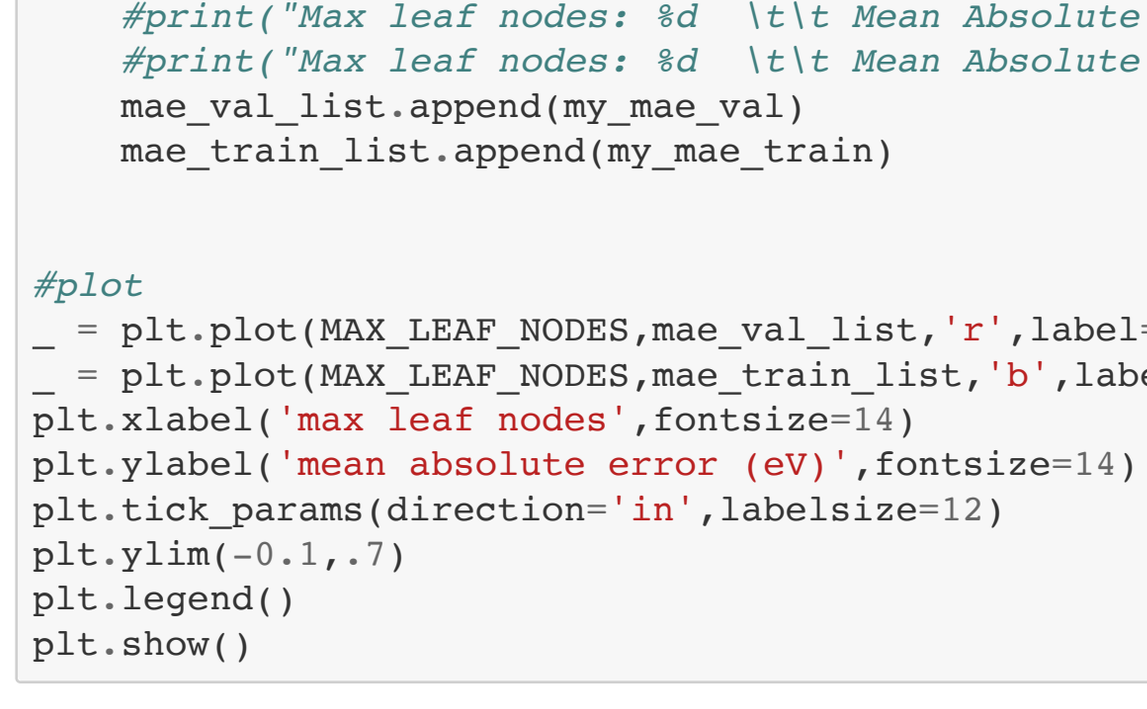
```
(5000, 2)
(5000, 9)
The ratio of MAE to the avg En value in the validation set is 1.5082859740195078e-05
mean_absolute_error using coord. as features is 0.4488
The ratio of MAE to the avg En value in the validation set is 2.2180676088522174e-05
mean_absolute_error using angles as features is 0.66
```

the mean absolute error is lower when using the water molecule coordinates as features. Hereon, I use coordinates of the water molecule as features.

Control Overfitting and Underfitting

In [16]:
```
def get_mae(train_X,train_y,val_X,val_y,max_leaf_nodes):

    Model = DecisionTreeClassifier(max_leaf_nodes=max_leaf_nodes,random_state=0)
    Model.fit(train_X,train_y)
    pred_vals = Model.predict(val_X)
    pred_val_train = Model.predict(train_X)
    mae_val = mean_absolute_error(val_y,pred_vals)
    mae_train = mean_absolute_error(train_y,pred_val_train)

    return mae_val, mae_train
```

In [17]:
```
MAX_LEAF_NODES = range(2,800,5)
mae_val_list = []
mae_train_list = []

for max_leaf_nodes in MAX_LEAF_NODES:
    my_mae_val, my_mae_train = get_mae(train_X,train_y,val_X,val_y,max_leaf_nodes)
    #print("Max leaf nodes: %d  \t\t Mean Absolute validation Error:  %.3f" %(max_leaf_nodes, my_mae_val))
    #print("Max leaf nodes: %d  \t\t Mean Absolute training Error:  %.3f" %(max_leaf_nodes, my_mae_train))
    mae_val_list.append(my_mae_val)
    mae_train_list.append(my_mae_train)


#plot
_ = plt.plot(MAX_LEAF_NODES,mae_val_list,'r',label='validation')
_ = plt.plot(MAX_LEAF_NODES,mae_train_list,'b',label='training')
plt.xlabel('max leaf nodes',fontsize=14)
plt.ylabel('mean absolute error (eV)',fontsize=14)
plt.tick_params(direction='in',labelsize=12)
plt.ylim(-0.1,.7)
plt.legend()
plt.show()
```



In [18]:
```
mae_min = 10
best_tree_size = MAX_LEAF_NODES[0]

# find the ideal tree size from candidate_max_leaf_nodes
for max_leaf_nodes in MAX_LEAF_NODES:
    mae = get_mae(train_X,train_y,val_X,val_y,max_leaf_nodes)[0]
    if mae < mae_min:
        mae_min = mae
        best_tree_size = max_leaf_nodes

print(best_tree_size)


if __name__=='__main__':

    features = coords
    X = data[coords]
    yc = y_kmeans4

    train_X, val_X, train_y, val_y = train_test_split(X, yc, test_size=0.25, random_state=0)
    MAE, Rel_MAE,y_predict,y_score = MyTree(train_X,val_X,train_y,val_y,randomstate=1,
                                            max_leaf_nodes=best_tree_size)

    print("mean_absolute_error of the optimized tree using coord. as features is {}".format(MAE))
```

```
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The ratio of MAE to the avg En value in the validation set is 1.4437603708528978e-05
mean_absolute_error of the optimized tree using coord. as features is 0.4296
```
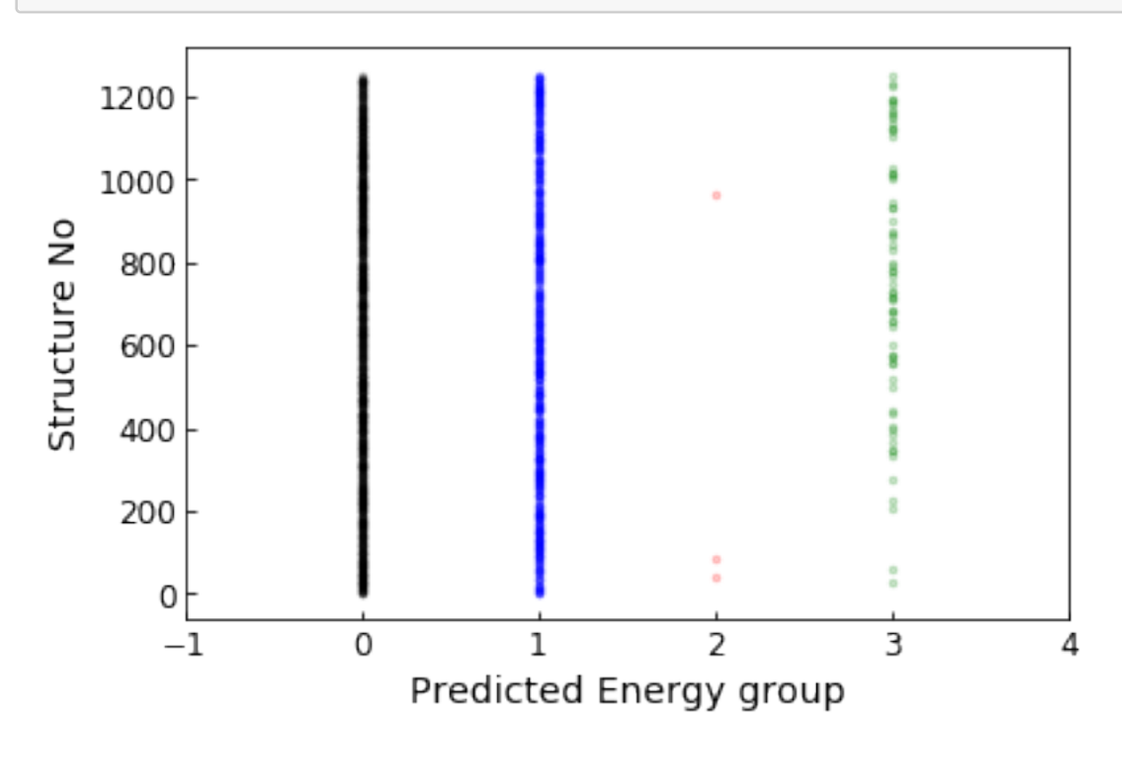

In [19]:
```
plt.figure()
plt.xlim(-1,np.max(y_predict)+1)
Configs = np.arange(0,1250)
bounds = [-29757, -29749.5, -29736]

cmap = ['k','b','r','g']
for i,y in enumerate(y_predict):
    plt.scatter(y, Configs[i], c=cmap[y], s=6.5, alpha=.2)

plt.xlabel(('Predicted Energy group'),fontsize=14)
plt.ylabel('Structure No',fontsize=14)
plt.tick_params(direction='in',labelsize=12)
plt.show()
```



We can see that the prediction is more accurate for the two lowest energy groups of data. However, for the other two energy groups, where the data is more sparsed, the model does not perform as well even after optimization.