Example 2: Learning crystal energy

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The main objective of this example is to get a small dataset of atomic crystal structures and their energy, fingerprint them, and develop some ML models using different learning algorithms.

1. Download data

The dataset contains 329 equilibrium structures of 13 different stoichiometries of Mg and Si, whose energy was computed using DFT. This dataset was reported in [T. D. Huan, *Pressure-stabilized binary compounds of magnesium and silicon*, Phys. Rev. Materials **2**, 023803 (2018)]. It will be obtained from www.matsml.org. More information on the avaiable datasets can be found at www.matsml.org as well.

In [1]:
```python
from matsml.data import Datasets
import os
import pandas as pd

# Load data
ds_name='crystals_MgSi_329'
data=Datasets(ds_name=ds_name)
data.load_dataset()

# have a look at the content
print (pd.read_csv(os.path.join(os.getcwd(),str(ds_name),'summary.csv')))
```

```
 matsML, version 1.0
 *****
 Load requested dataset(s)
   Data saved in crystals_MgSi_329
                 file_name     target
0    mg2si_struct_01.vasp  -8.924797
1    mg2si_struct_02.vasp -34.985707
2    mg2si_struct_03.vasp -17.246812
3    mg2si_struct_04.vasp -34.062642
4    mg2si_struct_05.vasp -34.035175
..                    ...        ...
324   mgsi_struct_30.vasp -40.698471
325   mgsi_struct_31.vasp -40.598719
326   mgsi_struct_32.vasp -40.499177
327   mgsi_struct_33.vasp  -6.706034
328   mgsi_struct_34.vasp -40.362384

[329 rows x 2 columns]
```

2. Fingerprint the obtained data

Two kinds of crystal fingerprints will be used in this example

1. Ewald sum matrix [Fe. Faber, A. Lindmaa, O. Anatole von Lilienfeld, and R. Armiento. *Crystal structure representations for machine learning models of formation energies* Int. J. Quantum Chem., 115, 1094 (2015)] is an analogy to the Coulomb matrix for molecules, and its size also depends on the number of atoms of the structure. We used a similar projection on a set of Gaussian. Keyword for this fingerprint is **pesm_crystals**.
2. Smooth Overlap of Atomic Positions (SOAP) [S. De, A. P. Bartók, G. Csányi, and M. Ceriotti, *Comparing molecules and solids across structural and alchemical space*, Phys. Chem. Chem. Phys. **18**, 13754 (2016)] is a more sophisticated fingerprint. Keyword for this fingerprint is **soap_crystals**.

In [2]:
```python
import pandas as pd
from matsml.fingerprint import Fingerprint

summary=os.path.join(os.getcwd(),'crystals_MgSi_329/summary.csv')
data_loc=os.path.join(os.getcwd(),'crystals_MgSi_329')
n_atoms_max=28                          # Max number of atoms in all the structures
fp_dim=20                               # intended fingerprint dimensionality
verbosity=0                             # verbosity, 0 or 1
species=['Mg','Si']

# Edwald sum matrix
data_params_pesm={'summary':summary,'data_loc':data_loc,'fp_file':'fp_crystals_MgSi_329_pesm.csv',
    'fp_type':'pesm_crystals','fp_dim':fp_dim,'verbosity':verbosity,
    'n_atoms_max':n_atoms_max,'species':species}

fp_pesm=Fingerprint(data_params_pesm)
fp_pesm.get_fingerprint()

# SOAP
data_params_soap={'summary':summary,'data_loc':data_loc,'fp_file':'fp_crystals_MgSi_329_soap.csv',
    'fp_type':'soap_crystals','fp_dim':fp_dim,'verbosity':verbosity,
    'n_atoms_max':n_atoms_max,'species':species}
fp_pesm=Fingerprint(data_params_soap)
fp_pesm.get_fingerprint()
```

```
 Atomic structure fingerprinting
   summary                     /home/huan/work/matsml/examples/ex2_crystals/crystals_MgSi_329/summary.csv
   data_loc                    /home/huan/work/matsml/examples/ex2_crystals/crystals_MgSi_329
   species                     ['Mg', 'Si']
   fp_type                     pesm_crystals
   fp_file                     fp_crystals_MgSi_329_pesm.csv
   fp_dim                      20
   n_atoms_max                 28
   verbosity                   0
 Read input
   num_structs                 329
 Computing Ewald sum Matrix
   [==                                                ] 3%
/home/huan/miniconda3/envs/tf/lib/python3.8/site-packages/ase/utils/__init__.py:62: FutureWarning: Please use a
toms.cell.reciprocal()
  warnings.warn(warning)
   [==================================================] 100%
 Projecting Ewald sum matrix to create fingerprints
   [==================================================] 100%
 Done fingerprinting, results saved in fp_crystals_MgSi_329_pesm.csv
 Atomic structure fingerprinting
   summary                     /home/huan/work/matsml/examples/ex2_crystals/crystals_MgSi_329/summary.csv
   data_loc                    /home/huan/work/matsml/examples/ex2_crystals/crystals_MgSi_329
   species                     ['Mg', 'Si']
   fp_type                     soap_crystals
   fp_file                     fp_crystals_MgSi_329_soap.csv
   fp_dim                      20
   n_atoms_max                 28
   verbosity                   0
 Read input
   num_structs                 329
 Computing SOAP fingerprint
   [==================================================] 100%
 Done fingerprinting, results saved in fp_crystals_MgSi_329_soap.csv
```

The fingerprinting step maybe a bit slow for a tutorial because we need to set n_atoms_max=28, which results in quite large Ewald sum matricies. A version of fingerprinted data can also be obtained in case you want to skip this step.

In [3]:
```python
from matsml.data import Datasets
import os
import pandas as pd

# Load data
data=Datasets(ds_soap='fp_crystals_MgSi_329_soap', ds_pesm='fp_crystals_MgSi_329_pesm')
data.load_dataset()

print (os.path.isfile('fp_crystals_MgSi_329_soap.csv.gz'))
print (os.path.isfile('fp_crystals_MgSi_329_pesm.csv.gz'))
```

```
 Load requested dataset(s)
   Data saved in fp_crystals_MgSi_329_soap.csv.gz
   Data saved in fp_crystals_MgSi_329_pesm.csv.gz
True
True
```

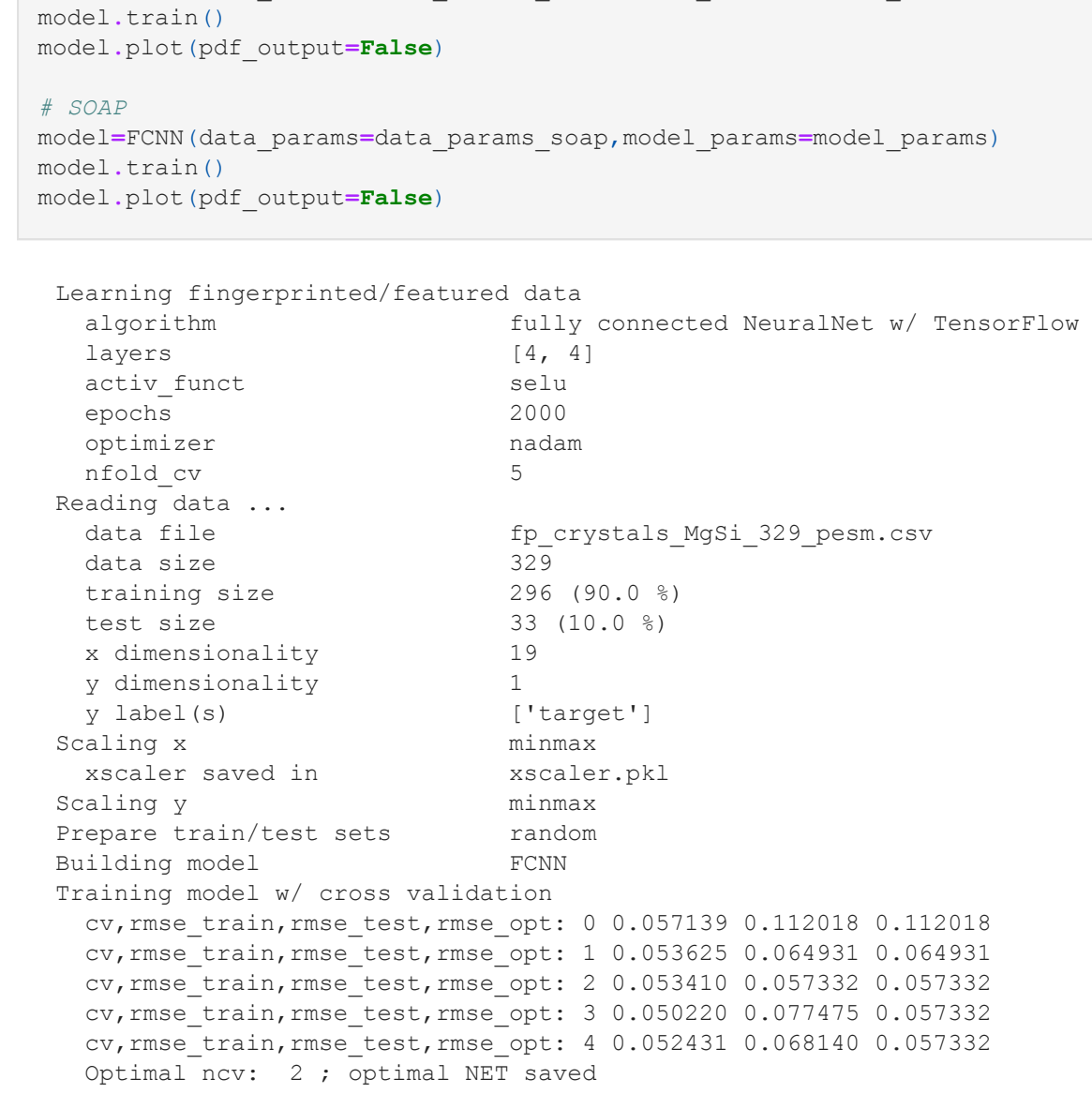
3. Train several ML models with two finterprint files just created

In [4]:
```python
# data parameters for learning

id_col=['id']                            # this is id column in the fingerprint data
y_cols=['target']                        # this is y columns
comment_cols=[]                          # other columns that are not id, not x, nor y columns
n_trains=0.9                             # 90% for training, 15% for validating
sampling='random'                        # way of train/test spliting. Random and more
x_scaling='minmax'
y_scaling='minmax'

data_params_pesm={'data_file':'fp_crystals_MgSi_329_pesm.csv','id_col':id_col,
    'y_cols':y_cols,'comment_cols':comment_cols,'y_scaling':y_scaling,
    'x_scaling':x_scaling,'sampling':sampling, 'n_trains':n_trains}

data_params_soap={'data_file':'fp_crystals_MgSi_329_soap.csv','id_col':id_col,
    'y_cols':y_cols,'comment_cols':comment_cols,'y_scaling':y_scaling,
    'x_scaling':x_scaling,'sampling':sampling, 'n_trains':n_trains}
```

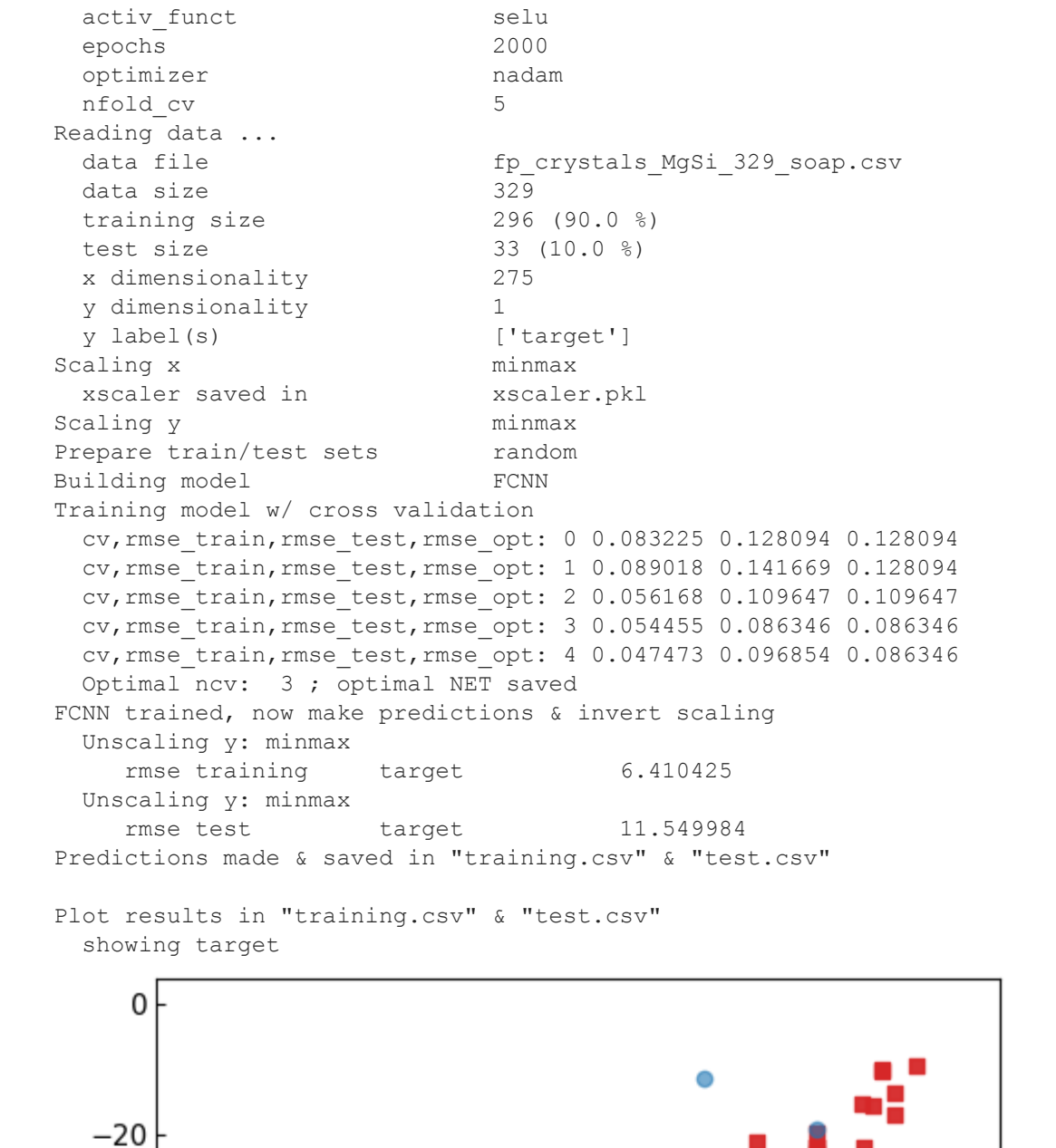
3a. Fully-connected NeuralNet

In [5]:
```python
from matsml.models import FCNN

# Model parameters
layers=[4,4]                   # list of nodes in hidden layers
epochs=2000                    # Epochs
nfold_cv=5                     # Number of folds for cross validation
use_bias=True                  # Use bias term or not
model_file='model_nn.pkl'      # Name of the model file to be created
verbosity=0                    # Verbosity, 0 or 1
batch_size=32                  # Default = 32
loss='mse'
activ_funct='selu'             # Options: "tanh", "relu", and more
optimizer='nadam'              # options: "Nadam", "Adam", and more

model_params={'layers':layers,'activ_funct':activ_funct,'epochs':epochs,
    'nfold_cv':nfold_cv,'optimizer':optimizer,'use_bias':use_bias,
    'model_file':model_file,'loss':loss,'batch_size':batch_size,
    'verbosity':verbosity,'rmse_cv':False}

# PESM
model=FCNN(data_params=data_params_pesm,model_params=model_params)
model.train()
model.plot(pdf_output=False)

# SOAP
model=FCNN(data_params=data_params_soap,model_params=model_params)
model.train()
model.plot(pdf_output=False)
```

```
 Learning fingerprinted/featured data
   algorithm                   fully connected NeuralNet w/ TensorFlow
   layers                      [4, 4]
   activ_funct                 selu
   epochs                      2000
   optimizer                   nadam
   nfold_cv                    5
 Reading data ...
   data file                   fp_crystals_MgSi_329_pesm.csv
   data size                   329
   training size               296 (90.0 %)
   test size                   33 (10.0 %)
   x dimensionality            19
   y dimensionality            1
   y label(s)                  ['target']
 Scaling x                     minmax
   xscaler saved in            xscaler.pkl
 Scaling y                     minmax
 Prepare train/test sets       random
 Building model                FCNN
 Training model w/ cross validation
   cv,rmse_train,rmse_test,rmse_opt: 0 0.057139 0.112018 0.112018
   cv,rmse_train,rmse_test,rmse_opt: 1 0.053625 0.064931 0.064931
   cv,rmse_train,rmse_test,rmse_opt: 2 0.053410 0.057332 0.057332
   cv,rmse_train,rmse_test,rmse_opt: 3 0.050220 0.077475 0.057332
   cv,rmse_train,rmse_test,rmse_opt: 4 0.052431 0.068140 0.057332
   Optimal ncv:  2 ; optimal NET saved
 FCNN trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           5.593569
   Unscaling y: minmax
      rmse test         target           6.593224
 Predictions made & saved in "training.csv" & "test.csv"

 Plot results in "training.csv" & "test.csv"
   showing target
```



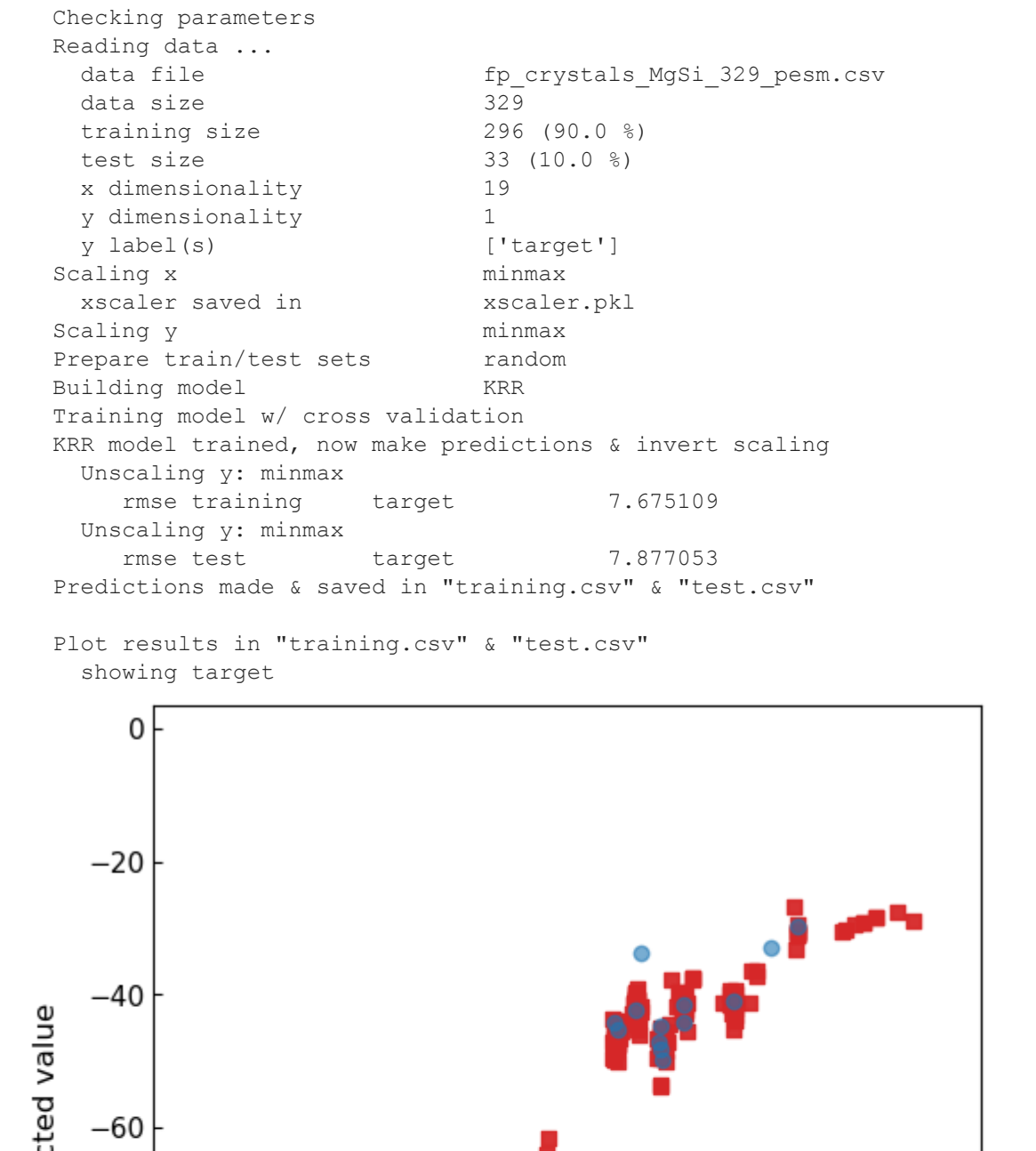

```
 Learning fingerprinted/featured data
   algorithm                   fully connected NeuralNet w/ TensorFlow
   layers                      [4, 4]
   activ_funct                 selu
   epochs                      2000
   optimizer                   nadam
   nfold_cv                    5
 Reading data ...
   data file                   fp_crystals_MgSi_329_soap.csv
   data size                   329
   training size               296 (90.0 %)
   test size                   33 (10.0 %)
   x dimensionality            275
   y dimensionality            1
   y label(s)                  ['target']
 Scaling x                     minmax
   xscaler saved in            xscaler.pkl
 Scaling y                     minmax
 Prepare train/test sets       random
 Building model                FCNN
 Training model w/ cross validation
   cv,rmse_train,rmse_test,rmse_opt: 0 0.083225 0.128094 0.128094
   cv,rmse_train,rmse_test,rmse_opt: 1 0.089018 0.141669 0.128094
   cv,rmse_train,rmse_test,rmse_opt: 2 0.056168 0.109647 0.109647
   cv,rmse_train,rmse_test,rmse_opt: 3 0.054455 0.086346 0.086346
   cv,rmse_train,rmse_test,rmse_opt: 4 0.047473 0.096854 0.086346
   Optimal ncv:  3 ; optimal NET saved
 FCNN trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           6.410425
   Unscaling y: minmax
      rmse test         target           11.549984
 Predictions made & saved in "training.csv" & "test.csv"

 Plot results in "training.csv" & "test.csv"
   showing target
```



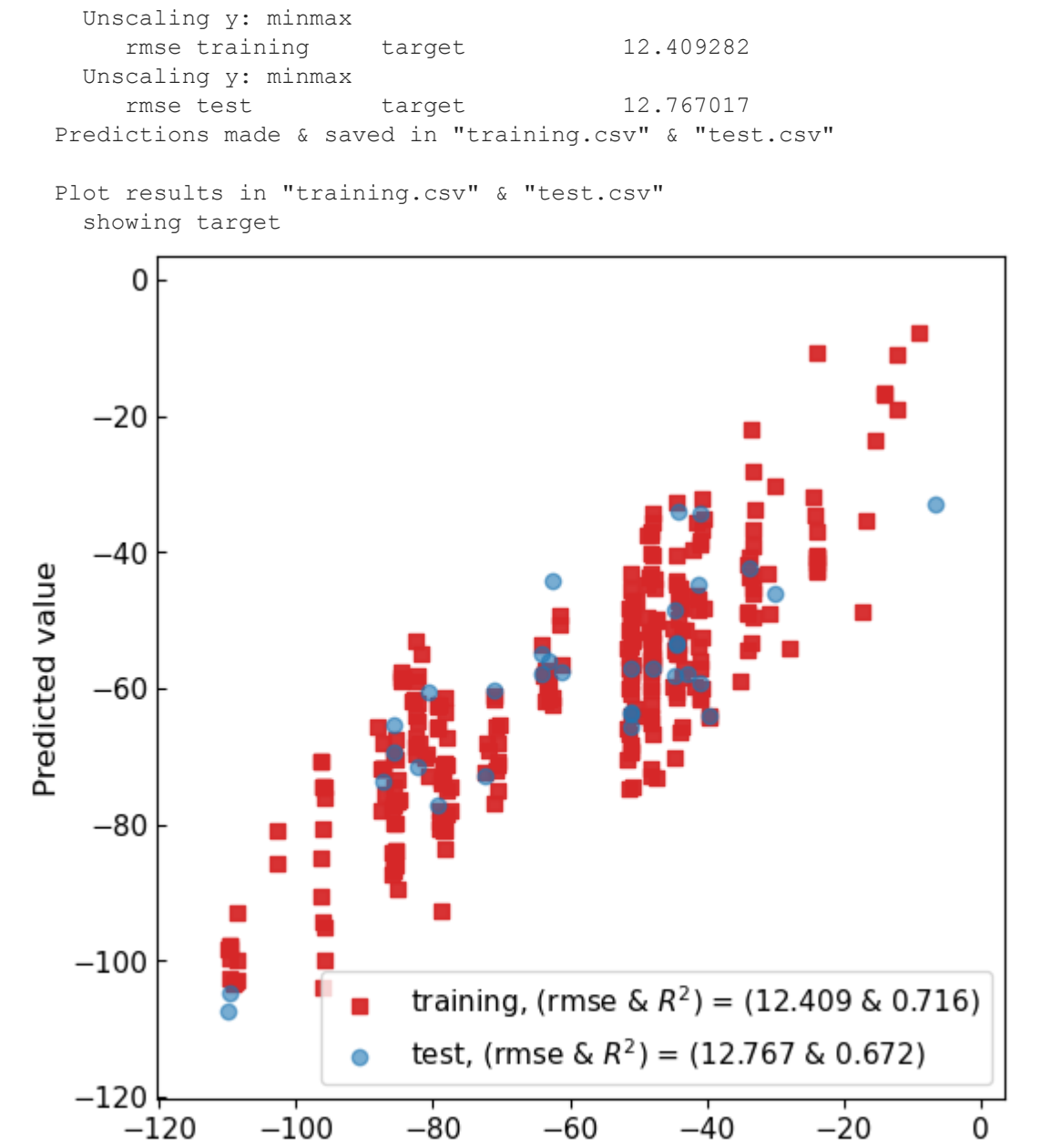
3b. KRR

In [6]:
```python
from matsml.models import KRR

# Model parameters
nfold_cv = 5                    # Number of folds for cross validation
model_file = 'model_krr.pkl'    # Name of the model file to be created
alpha = [-2,5]
gamma = [-2,5]
n_grids = 10
kernel = 'rbf'

model_params={'kernel':kernel,'nfold_cv':nfold_cv,'model_file':model_file,
              'alpha':alpha,'gamma':gamma,'n_grids':n_grids}

#PCM
model = KRR(data_params=data_params_pesm,model_params=model_params)
model.train()
model.plot(pdf_output=False)

#SOAP
model = KRR(data_params=data_params_soap,model_params=model_params)
model.train()
model.plot(pdf_output=False)
```

```
 Learning fingerprinted/featured data
   algorithm                   kernel ridge regression w/ scikit-learn
   kernel                      rbf
   nfold_cv                    5
   alpha                       [-2, 5]
   gamma                       [-2, 5]
   number of alpha/gamma grids 10
 Checking parameters
 Reading data ...
   data file                   fp_crystals_MgSi_329_pesm.csv
   data size                   329
   training size               296 (90.0 %)
   test size                   33 (10.0 %)
   x dimensionality            19
   y dimensionality            1
   y label(s)                  ['target']
 Scaling x                     minmax
   xscaler saved in            xscaler.pkl
 Scaling y                     minmax
 Prepare train/test sets       random
 Building model                KRR
 Training model w/ cross validation
 KRR model trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           7.675109
   Unscaling y: minmax
      rmse test         target           7.877053
 Predictions made & saved in "training.csv" & "test.csv"

 Plot results in "training.csv" & "test.csv"
   showing target
```



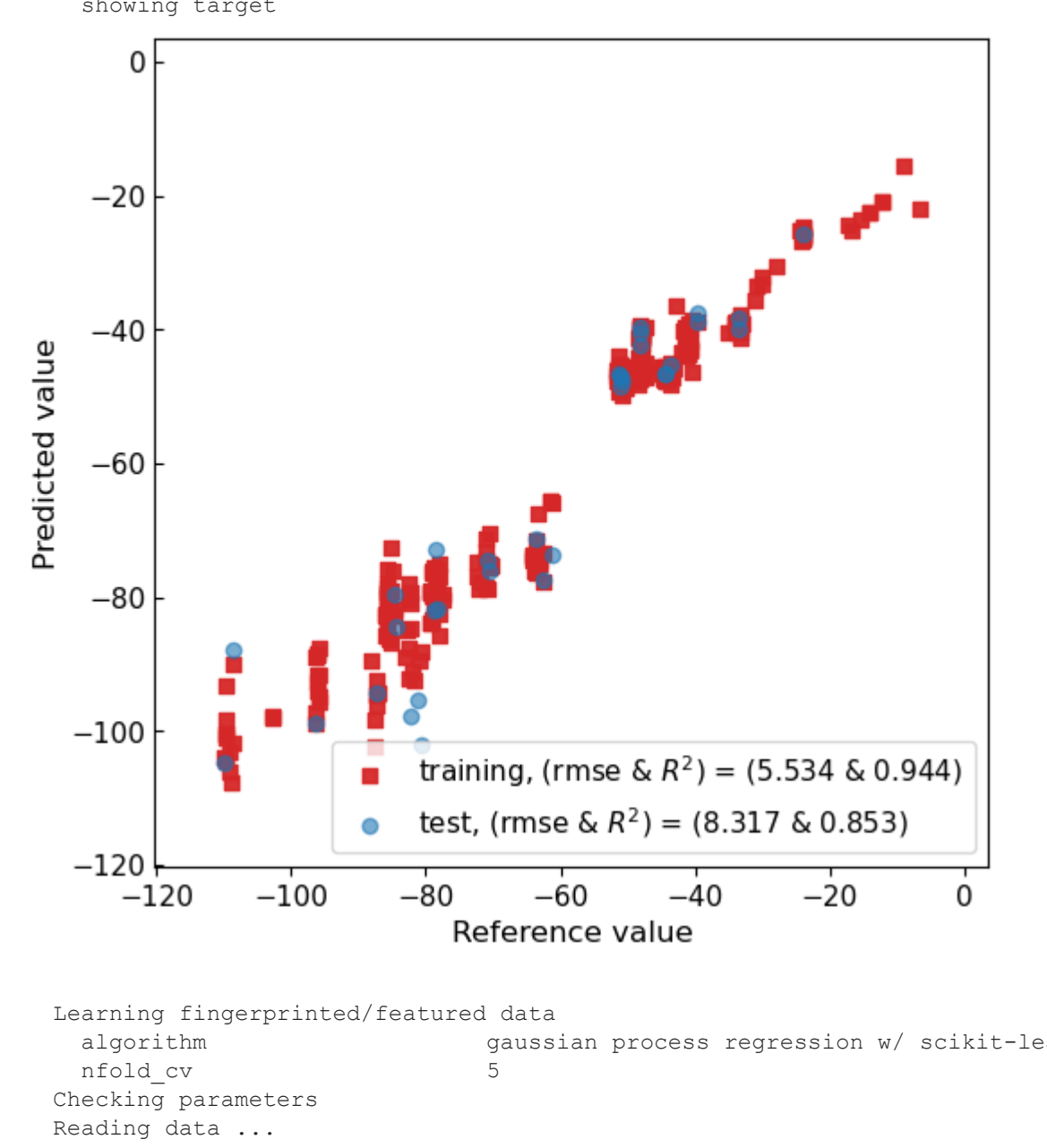

```
 Learning fingerprinted/featured data
   algorithm                   kernel ridge regression w/ scikit-learn
   kernel                      rbf
   nfold_cv                    5
   alpha                       [-2, 5]
   gamma                       [-2, 5]
   number of alpha/gamma grids 10
 Checking parameters
 Reading data ...
   data file                   fp_crystals_MgSi_329_soap.csv
   data size                   329
   training size               296 (90.0 %)
   test size                   33 (10.0 %)
   x dimensionality            275
   y dimensionality            1
   y label(s)                  ['target']
 Scaling x                     minmax
   xscaler saved in            xscaler.pkl
 Scaling y                     minmax
 Prepare train/test sets       random
 Building model                KRR
 Training model w/ cross validation
 KRR model trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           12.409282
   Unscaling y: minmax
      rmse test         target           12.767017
 Predictions made & saved in "training.csv" & "test.csv"

 Plot results in "training.csv" & "test.csv"
   showing target
```



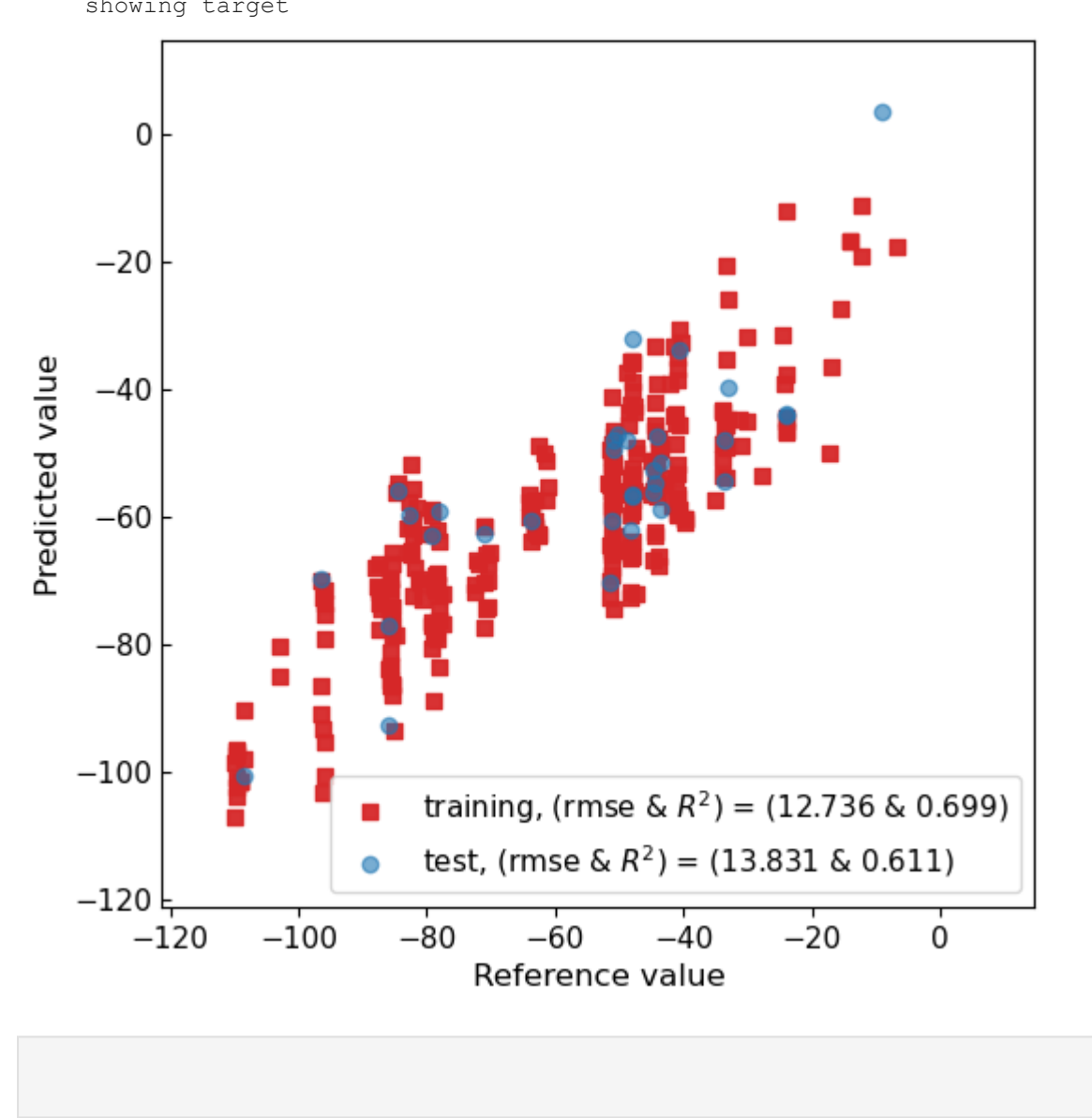
3c. GPR

In [7]:
```python
from matsml.models import GPR

# Model parameters
nfold_cv=5                      # Number of folds for cross validation
model_file='model_gpr.pkl'      # Name of the model file to be created
verbosity=0
rmse_cv=False
n_restarts_optimizer=200

model_params={'nfold_cv':nfold_cv,'n_restarts_optimizer':n_restarts_optimizer,
        'model_file':model_file,'verbosity':verbosity,'rmse_cv':rmse_cv}

#PCM
model=GPR(data_params=data_params_pesm,model_params=model_params)
model.train()
model.plot(pdf_output=False)

#SOAP
model=GPR(data_params=data_params_soap,model_params=model_params)
model.train()
model.plot(pdf_output=False)
```

```
 Learning fingerprinted/featured data
   algorithm                   gaussian process regression w/ scikit-learn
   nfold_cv                    5
 Checking parameters
 Reading data ...
   data file                   fp_crystals_MgSi_329_pesm.csv
   data size                   329
   training size               296 (90.0 %)
   test size                   33 (10.0 %)
   x dimensionality            19
   y dimensionality            1
   y label(s)                  ['target']
 Scaling x                     minmax
   xscaler saved in            xscaler.pkl
 Scaling y                     minmax
 Prepare train/test sets       random
 Training model w/ cross validation
   cv,rmse_train,rmse_test,rmse_opt: 0 0.054438 0.072064 0.072064
   cv,rmse_train,rmse_test,rmse_opt: 1 0.044269 0.078539 0.072064
   cv,rmse_train,rmse_test,rmse_opt: 2 0.052521 0.084744 0.072064
   cv,rmse_train,rmse_test,rmse_opt: 3 0.047645 0.068950 0.068950
   cv,rmse_train,rmse_test,rmse_opt: 4 0.054349 0.076845 0.068950
 GPR model trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           5.534074
   Unscaling y: minmax
      rmse test         target           8.316883
 Predictions made & saved in "training.csv" & "test.csv"

 Plot results in "training.csv" & "test.csv"
   showing target
```




```
 Learning fingerprinted/featured data
   algorithm                   gaussian process regression w/ scikit-learn
   nfold_cv                    5
 Checking parameters
 Reading data ...
   data file                   fp_crystals_MgSi_329_soap.csv
   data size                   329
   training size               296 (90.0 %)
   test size                   33 (10.0 %)
   x dimensionality            275
   y dimensionality            1
   y label(s)                  ['target']
 Scaling x                     minmax
   xscaler saved in            xscaler.pkl
 Scaling y                     minmax
 Prepare train/test sets       random
 Training model w/ cross validation
   cv,rmse_train,rmse_test,rmse_opt: 0 0.118419 0.147128 0.147128
   cv,rmse_train,rmse_test,rmse_opt: 1 0.113514 0.144823 0.144823
   cv,rmse_train,rmse_test,rmse_opt: 2 0.104519 0.170750 0.144823
   cv,rmse_train,rmse_test,rmse_opt: 3 0.127369 0.149515 0.144823
   cv,rmse_train,rmse_test,rmse_opt: 4 0.124282 0.160096 0.144823
 GPR model trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           12.735629
   Unscaling y: minmax
      rmse test         target           13.831175
 Predictions made & saved in "training.csv" & "test.csv"

 Plot results in "training.csv" & "test.csv"
   showing target
```



In [ ]: