Example 2: Fingerprint atomic crystal structures and learning their 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]:
```
from matsml.data import Datasets
import os
import pandas as pd

# Load data
ds_name='crystals_MgSi'
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 1.0.0
  *****
  Load requested dataset(s)
    Data saved in crystals_MgSi
                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. Different from the Ewald sum matrix which is defined for the whole system, SOAP is defined for each atom. Herein, for simplicity, the atomic fingerprints are added up to make the fingerprint for the whole system. In some ML potential, the SOAP fingerprints are used in a different way, involving the "atomic energy". The keyword for SOAP in matsML is **soap_crystals**.

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

summary=os.path.join(os.getcwd(),'crystals_MgSi/summary.csv')
data_loc=os.path.join(os.getcwd(),'crystals_MgSi')
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_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_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/ex3_crystals/crystals_MgSi/summary.csv
    data_loc                    /home/huan/work/matsml_examples/ex3_crystals/crystals_MgSi
    species                     ['Mg', 'Si']
    fp_type                     pesm_crystals
    fp_file                     fp_crystals_MgSi_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_pesm.csv
  Atomic structure fingerprinting
    summary                     /home/huan/work/matsml_examples/ex3_crystals/crystals_MgSi/summary.csv
    data_loc                    /home/huan/work/matsml_examples/ex3_crystals/crystals_MgSi
    species                     ['Mg', 'Si']
    fp_type                     soap_crystals
    fp_file                     fp_crystals_MgSi_soap.csv
    fp_dim                      20
    n_atoms_max                 28
    verbosity                   0
  Read input
    num_structs                 329
  Computing SOAP fingerprint with DScribe
    [==================================================] 100%
  Done fingerprinting, results saved in fp_crystals_MgSi_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]:
```
from matsml.data import Datasets
import os
import pandas as pd

# Load data
data=Datasets(ds_soap='fp_crystals_MgSi_soap', ds_pesm='fp_crystals_MgSi_pesm')
data.load_dataset()

print (os.path.isfile('fp_crystals_MgSi_soap.csv.gz'))
print (os.path.isfile('fp_crystals_MgSi_pesm.csv.gz'))
```

```
  Load requested dataset(s)
    Data saved in fp_crystals_MgSi_soap.csv.gz
    Data saved in fp_crystals_MgSi_pesm.csv.gz
True
True
```

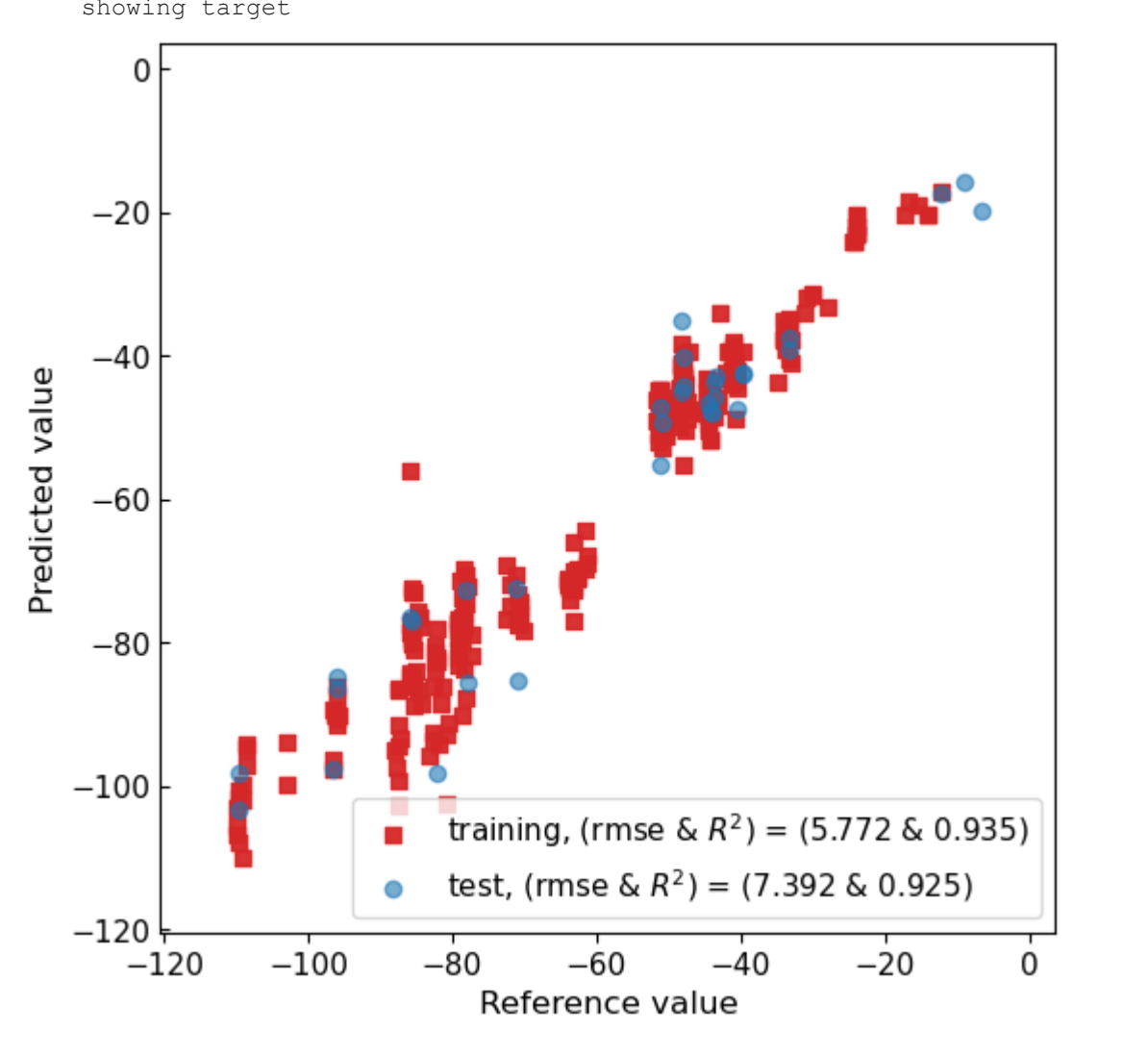
3. Train several ML models with two fingerprint files just created

In [4]:
```
# 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_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_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}
```

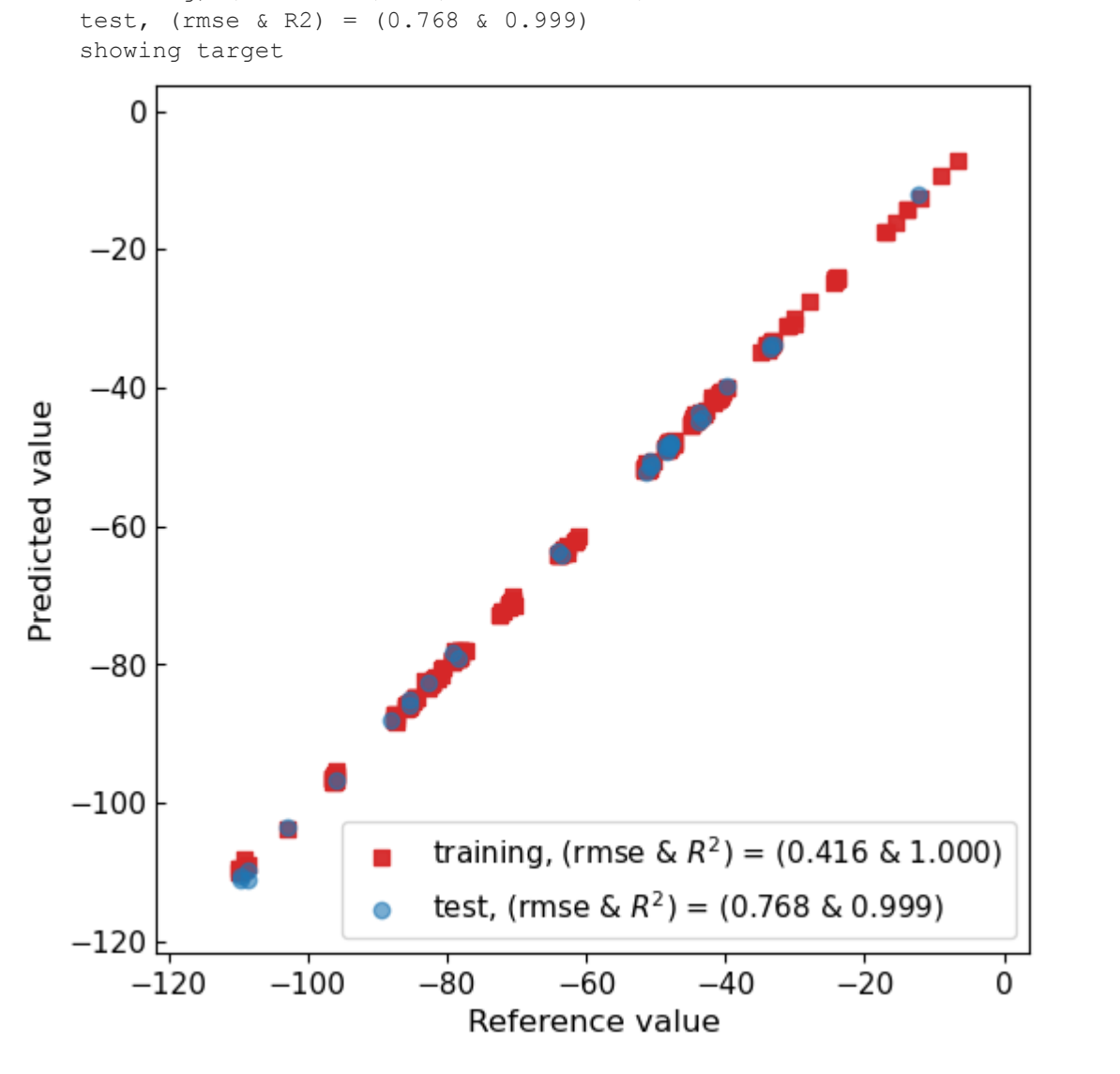
3a. Fully-connected NeuralNet

In [5]:
```
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
  Checking parameters
    all passed                  True
  Read data
    data file                   fp_crystals_MgSi_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 0.059275 0.072458 0.072458
    cv,rmse_train,rmse_test,rmse_opt: 1 0.055568 0.068262 0.068262
    cv,rmse_train,rmse_test,rmse_opt: 2 0.052195 0.066476 0.066476
    cv,rmse_train,rmse_test,rmse_opt: 3 0.053062 0.066252 0.066252
    cv,rmse_train,rmse_test,rmse_opt: 4 0.049476 0.075581 0.066252
    Optimal ncv:  3 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           5.771572
    unscaling y: minmax
       rmse test         target           7.392264
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (5.772 & 0.935)
    test, (rmse & R2) = (7.392 & 0.925)
    showing target
```



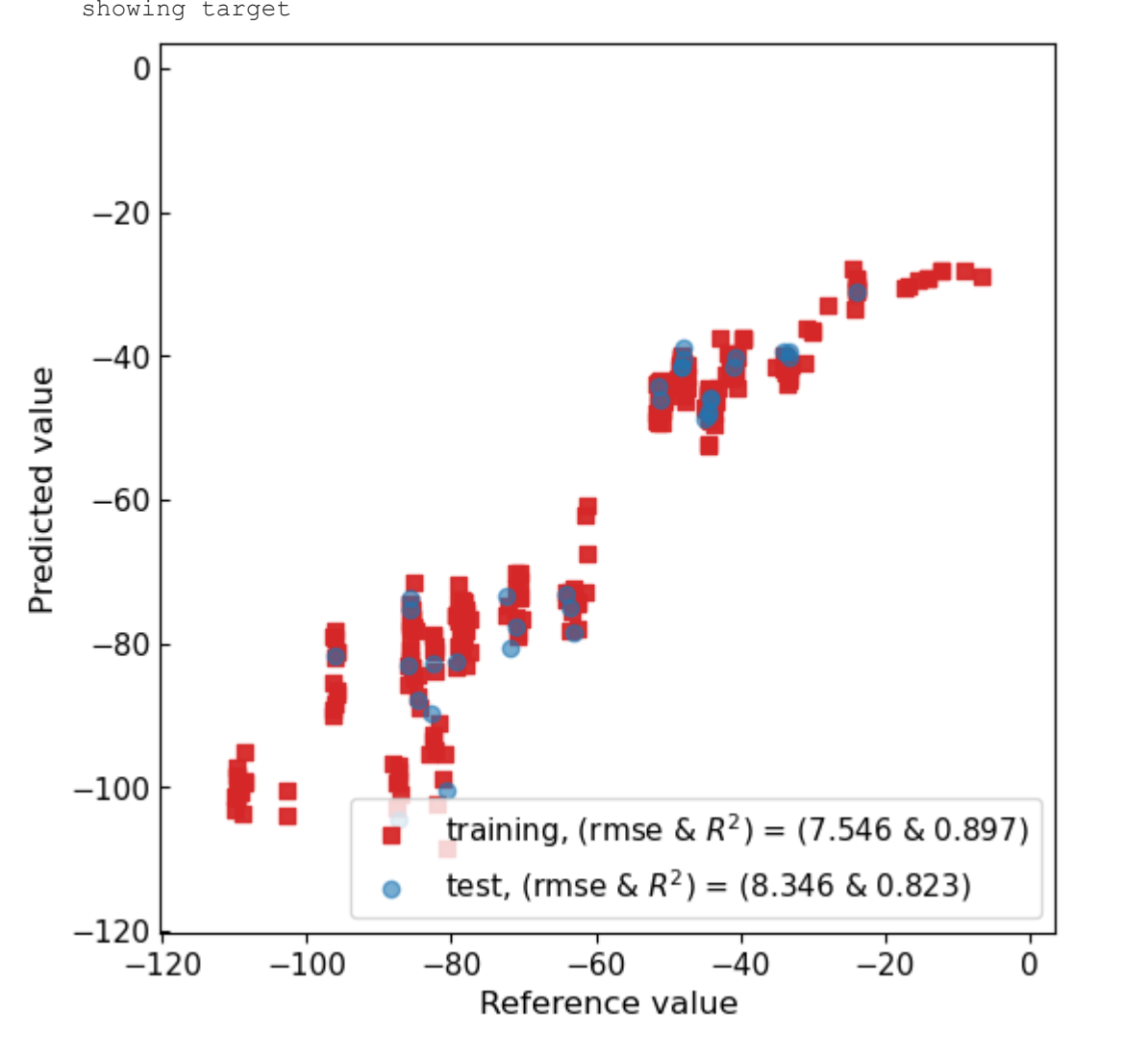

```
  Learning fingerprinted/featured data
    algorithm                   fully connected NeuralNet w/ TensorFlow
    layers                      [4, 4]
    activ_funct                 selu
    epochs                      2000
    optimizer                   nadam
    nfold_cv                    5
  Checking parameters
    all passed                  True
  Read data
    data file                   fp_crystals_MgSi_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 0.008504 0.009348 0.009348
    cv,rmse_train,rmse_test,rmse_opt: 1 0.009407 0.011897 0.009348
    cv,rmse_train,rmse_test,rmse_opt: 2 0.003605 0.005141 0.005141
    cv,rmse_train,rmse_test,rmse_opt: 3 0.003943 0.004369 0.004369
    cv,rmse_train,rmse_test,rmse_opt: 4 0.004335 0.006089 0.004369
    Optimal ncv:  3 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           0.415957
    unscaling y: minmax
       rmse test         target           0.767768
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.416 & 1.000)
    test, (rmse & R2) = (0.768 & 0.999)
    showing target
```



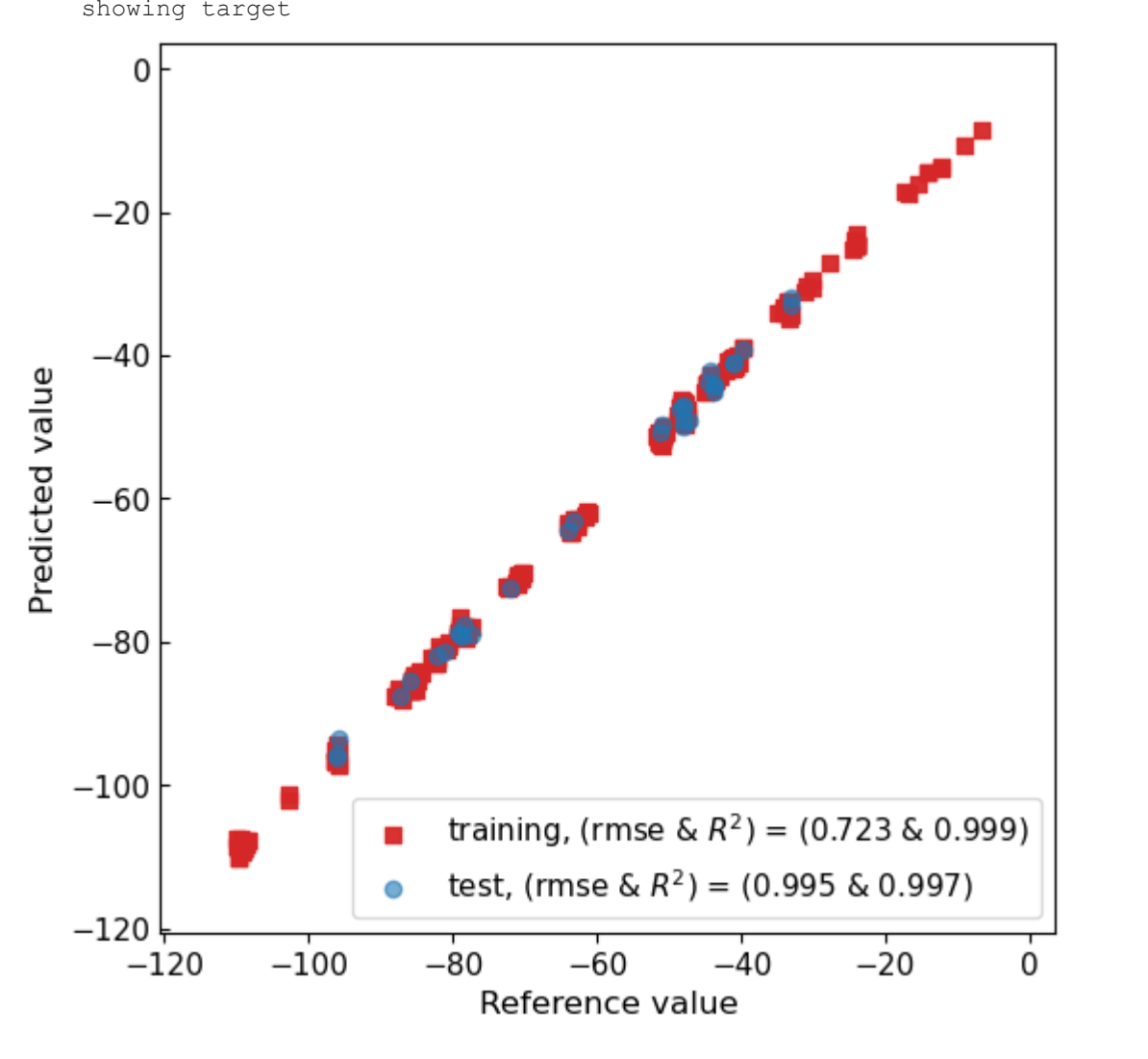
3b. KRR

In [6]:
```
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
    all passed                  True
  Read data
    data file                   fp_crystals_MgSi_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           7.546136
    unscaling y: minmax
       rmse test         target           8.345516
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (7.546 & 0.897)
    test, (rmse & R2) = (8.346 & 0.823)
    showing target
```



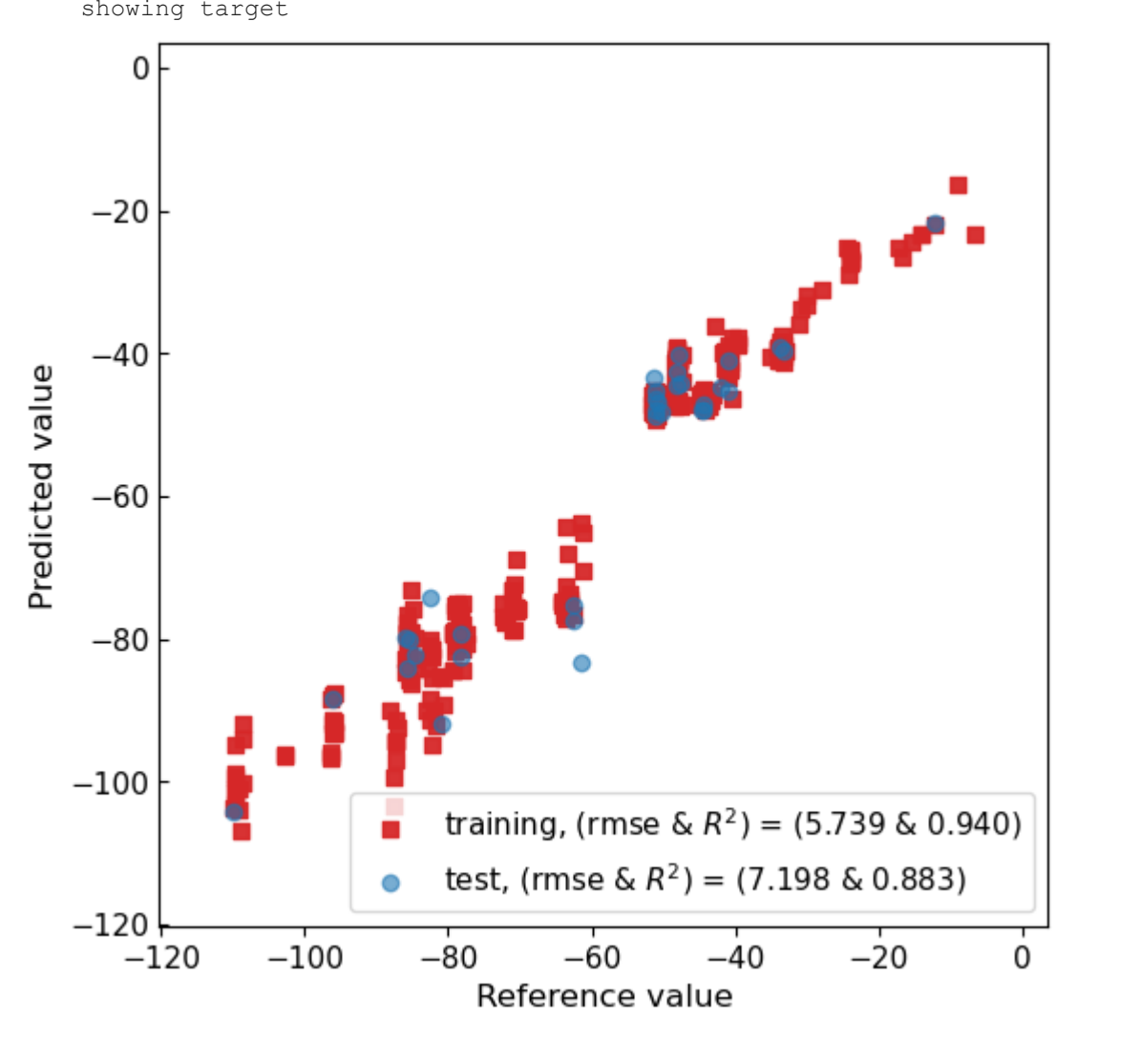

```
  Learning fingerprinted/featured data
    algorithm                   kernel ridge regression w/ scikit-learn
    kernel                      rbf
    nfold_cv                    5
    alpha                       [-2, 5]
    gamma                       [-2, 5]
    number of alpha/gamma grids 10
  Checking parameters
    all passed                  True
  Read data
    data file                   fp_crystals_MgSi_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           0.722876
    unscaling y: minmax
       rmse test         target           0.994546
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.723 & 0.999)
    test, (rmse & R2) = (0.995 & 0.997)
    showing target
```



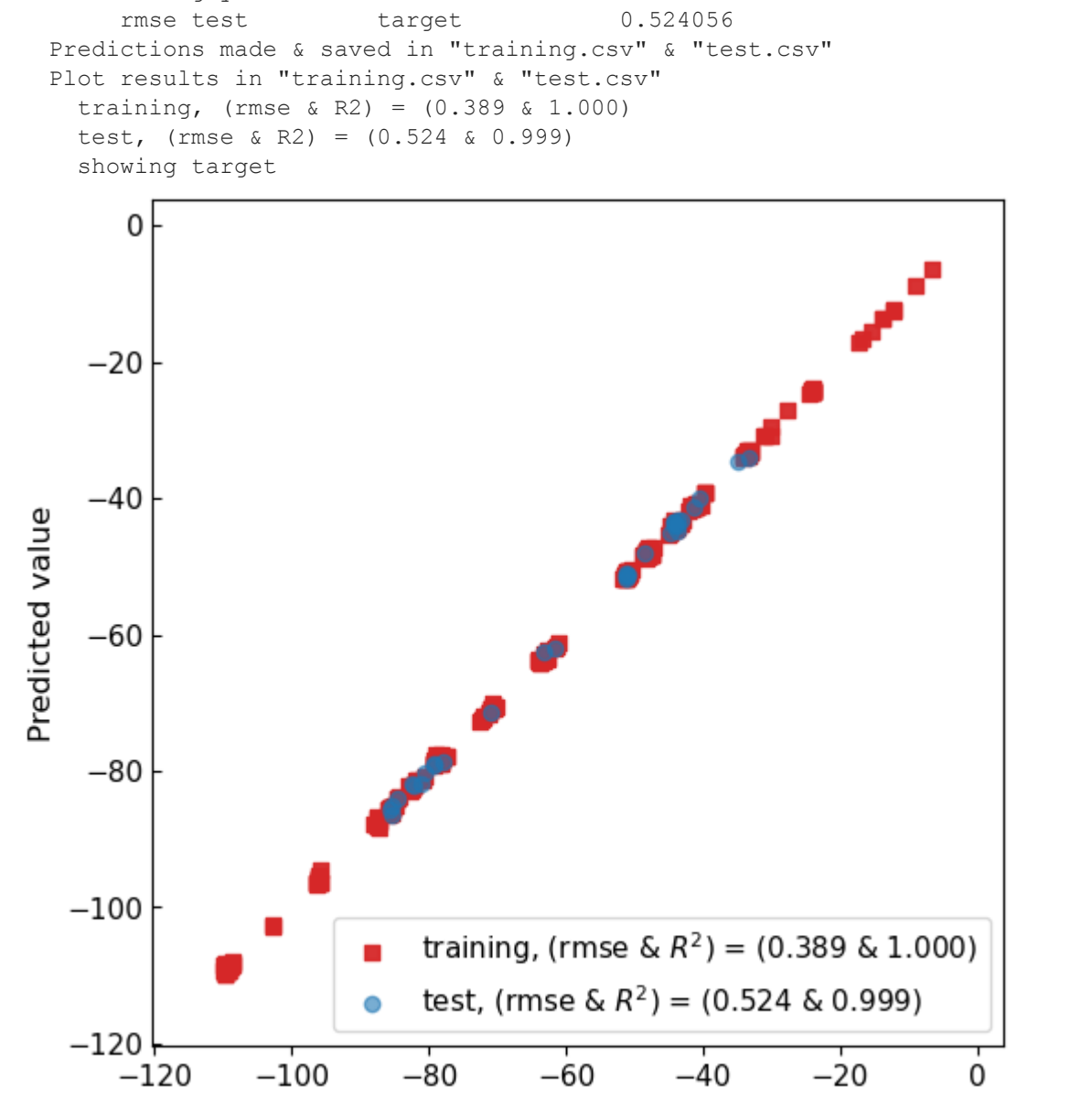
3c. GPR

In [7]:
```
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
    optimizer                   fmin_l_bfgs_b
    n_restarts_optimizer        200
    rmse_cv                     False
  Checking parameters
    all passed                  True
  Read data
    data file                   fp_crystals_MgSi_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 0.056704 0.064423 0.064423
    cv,rmse_train,rmse_test,rmse_opt: 1 0.055103 0.068148 0.064423
    cv,rmse_train,rmse_test,rmse_opt: 2 0.042161 0.079398 0.064423
    cv,rmse_train,rmse_test,rmse_opt: 3 0.057973 0.077506 0.064423
    cv,rmse_train,rmse_test,rmse_opt: 4 0.055984 0.070648 0.064423
  GPR model trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           5.738619
    unscaling y: minmax
       rmse test         target           7.19793
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (5.739 & 0.940)
    test, (rmse & R2) = (7.198 & 0.883)
    showing target
```




```
  Learning fingerprinted/featured data
    algorithm                   gaussian process regression w/ scikit-learn
    nfold_cv                    5
    optimizer                   fmin_l_bfgs_b
    n_restarts_optimizer        200
    rmse_cv                     False
  Checking parameters
    all passed                  True
  Read data
    data file                   fp_crystals_MgSi_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 0.003832 0.005269 0.005269
    cv,rmse_train,rmse_test,rmse_opt: 1 0.003830 0.006250 0.005269
    cv,rmse_train,rmse_test,rmse_opt: 2 0.004090 0.005269 0.005269
    cv,rmse_train,rmse_test,rmse_opt: 3 0.003853 0.005193 0.005193
    cv,rmse_train,rmse_test,rmse_opt: 4 0.003884 0.005324 0.005193
  GPR model trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           0.388807
    unscaling y: minmax
       rmse test         target           0.524056
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.389 & 1.000)
    test, (rmse & R2) = (0.524 & 0.999)
    showing target
```



In [ ]: