Example 1: Learning molecules energy

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The main objective of this example is to demonstrate a generic workflow of materials, involving (1) obtaining a small dataset of molecules and their energy, (2) fingerprint them, and (3) develop some ML models.

1. Download a dataset

The dataset contains 10,000 non-equilibrium structures of CH_3-NH-OH molecules, whose energy was computed using BigDFT package and HGH norm-conserving pseudopotentials. It is available at www.matsml.org.

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

# Load a dataset
dataset_name='molecs_CH3NHOH_10k'
data=Datasets(dataset_name=dataset_name)
data.load_dataset()

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

```
 matsML, version 1.0
 *****
 Load requested dataset(s)
   Data saved in molecs_CH3NHOH_10k
              file_name      target
0     CH3NHOH_00001.xyz -940.288539
1     CH3NHOH_00002.xyz -940.580380
2     CH3NHOH_00003.xyz -940.184809
3     CH3NHOH_00004.xyz -940.460977
4     CH3NHOH_00005.xyz -940.579457
...                 ...         ...
9994  CH3NHOH_09996.xyz -940.286083
9995  CH3NHOH_09997.xyz -940.744461
9996  CH3NHOH_09998.xyz -940.553979
9997  CH3NHOH_09999.xyz -940.650902
9998  CH3NHOH_10000.xyz -940.059079

[9999 rows x 2 columns]
```

2. Fingerprint the obtained data

Two kinds of fingerprints will be demonstrated here

1. Coulomb matrix (CM) [M. Rupp, A. Tkatchenko, K.-R. Müller, and O. Anatole von Lilienfeld, *Fast and accurate modeling of molecular atomization energies with machine learning*, Phys. Rev. Lett., 108, 058301 (2012)] is perhaps one of the earliest fingerprints used in materials informatics. It was defined as an $N \times N$ matrix for a molecule of N atoms. The key advantage of CM is that it is invariant under rotations and translations, required ro represent materials structure as a whole. However, its size depends on the molecule size, making it not directly usable for machine learning. Normally, the eigenvalues of these matricies are computed and sorted, and then zero padding is used to make fixed-size vectors. Here, we defined a projection of these Coulomb matricies onto a set of Gaussian functions, covering the entire range of the Coulomn matrix element values. The results are also a set of fixed-size fingerprints, which are ready for learning. Keyword for this fingerprint is **pcm_molecs**.
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_molecs**.

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

summary=os.path.join(os.getcwd(),'molecs_CH3NHOH_10k/summary.csv')
data_loc=os.path.join(os.getcwd(),'molecs_CH3NHOH_10k/')
n_atoms_max=8                          # max number of atoms in all of the structures to be fingerprinted
fp_dim=50                              # intended fingerprint dimensionality; the final number can be smaller
verbosity=0                            # verbosity, 0 or 1
species=['C','H', 'N', 'O']            # All the spacies in the datasets, used for SOAP

#PCM
data_params_pcm={'fp_type':'pcm_molecs','summary':summary,'data_loc':data_loc,
    'n_atoms_max':n_atoms_max,'fp_file':'fp_pcm.csv','fp_dim':fp_dim,
    'species':species,'verbosity':verbosity}

fp_pcm=Fingerprint(data_params_pcm)
fp_pcm.get_fingerprint()

# SOAP
data_params_soap={'fp_type':'soap_molecs','summary':summary,'data_loc':data_loc,
    'species':species,'n_atoms_max':n_atoms_max,'fp_file':'fp_soap.csv',
    'fp_dim':fp_dim,'verbosity':verbosity}

fp_soap=Fingerprint(data_params_soap)
fp_soap.get_fingerprint()
```

```
 Atomic structure fingerprinting
   summary                        /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH3NHOH_10k/summary.csv
   data_loc                       /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH3NHOH_10k/
   species                        ['C', 'H', 'N', 'O']
   fp_type                        pcm_molecs
   fp_file                        fp_pcm.csv
   fp_dim                         50
   n_atoms_max                    8
   verbosity                      0
 Read input
   num_structs                    9999
 Computing Coulomb matrix
   [==================================================] 100%
 Projecting Coulomb matrix to create fingerprints
   [==================================================] 100%
 Done fingerprinting, results saved in fp_pcm.csv
 Atomic structure fingerprinting
   summary                        /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH3NHOH_10k/summary.csv
   data_loc                       /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH3NHOH_10k/
   species                        ['C', 'H', 'N', 'O']
   fp_type                        soap_molecs
   fp_file                        fp_soap.csv
   fp_dim                         50
   n_atoms_max                    8
   verbosity                      0
 Read input
   num_structs                    9999
 Computing SOAP fingerprint
   [==================================================] 100%
 Done fingerprinting, results saved in fp_soap.csv
```

The fingerprinting step is slow. A version of fingerprinted data can also be obtained in case you want to skip this step. Pandas can read gzip files fo no need to unzip them.

In [3]:
```
from matsml.data import Datasets
import os

# Load data
data=Datasets(ds1='fp_molecs_CH3NHOH_10k_pcm',ds2='fp_molecs_CH3NHOH_10k_soap')
data.load_dataset()

print (os.path.isfile('fp_molecs_CH3NHOH_10k_pcm.csv.gz'))
print (os.path.isfile('fp_molecs_CH3NHOH_10k_soap.csv.gz'))
```

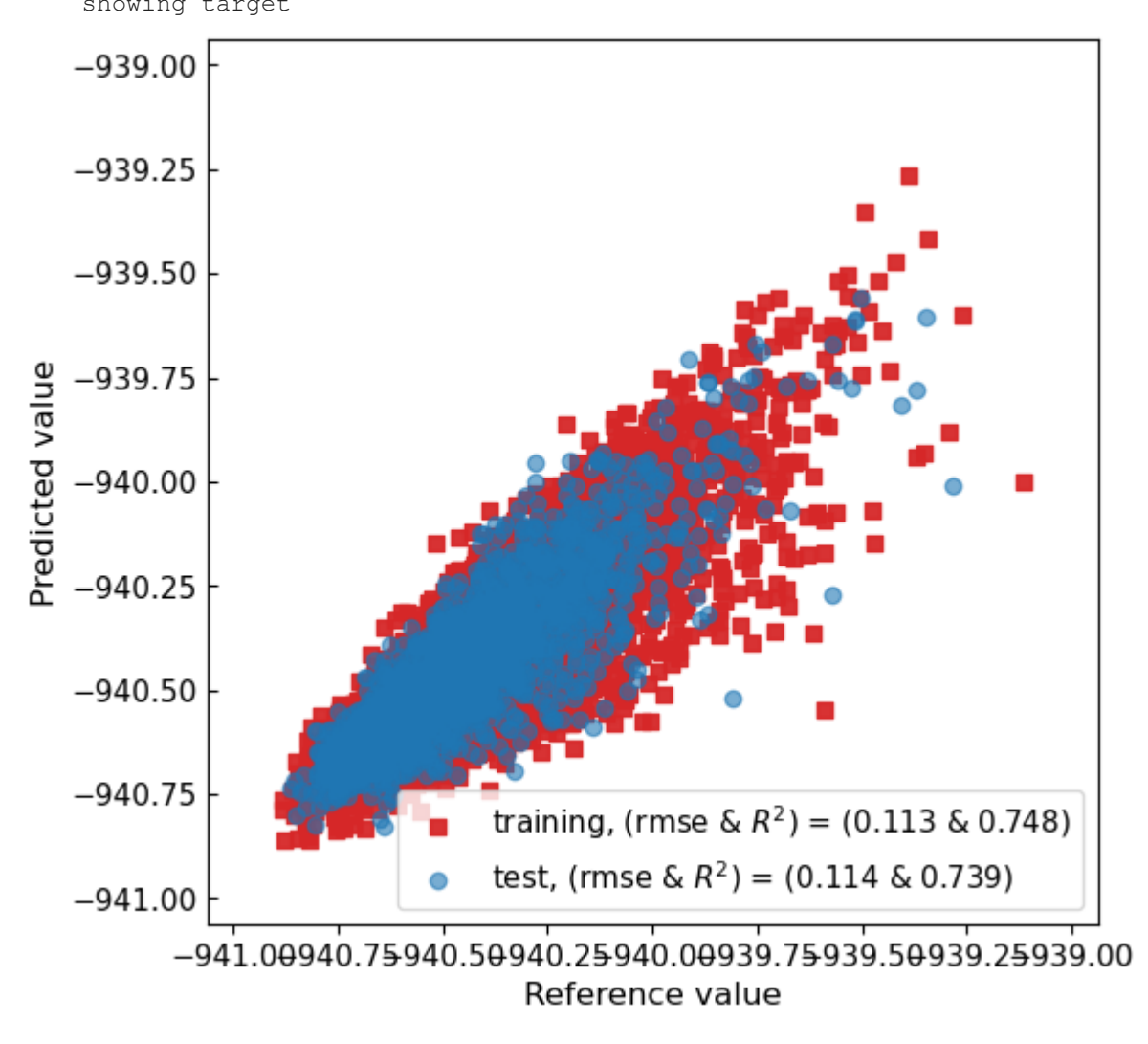
```
 Load requested dataset(s)
   Data saved in fp_molecs_CH3NHOH_10k_pcm.csv.gz
   Data saved in fp_molecs_CH3NHOH_10k_soap.csv.gz
True
True
```

3. Train some ML models with "fp_pcm.csv" and "fp_soap.csv" just created

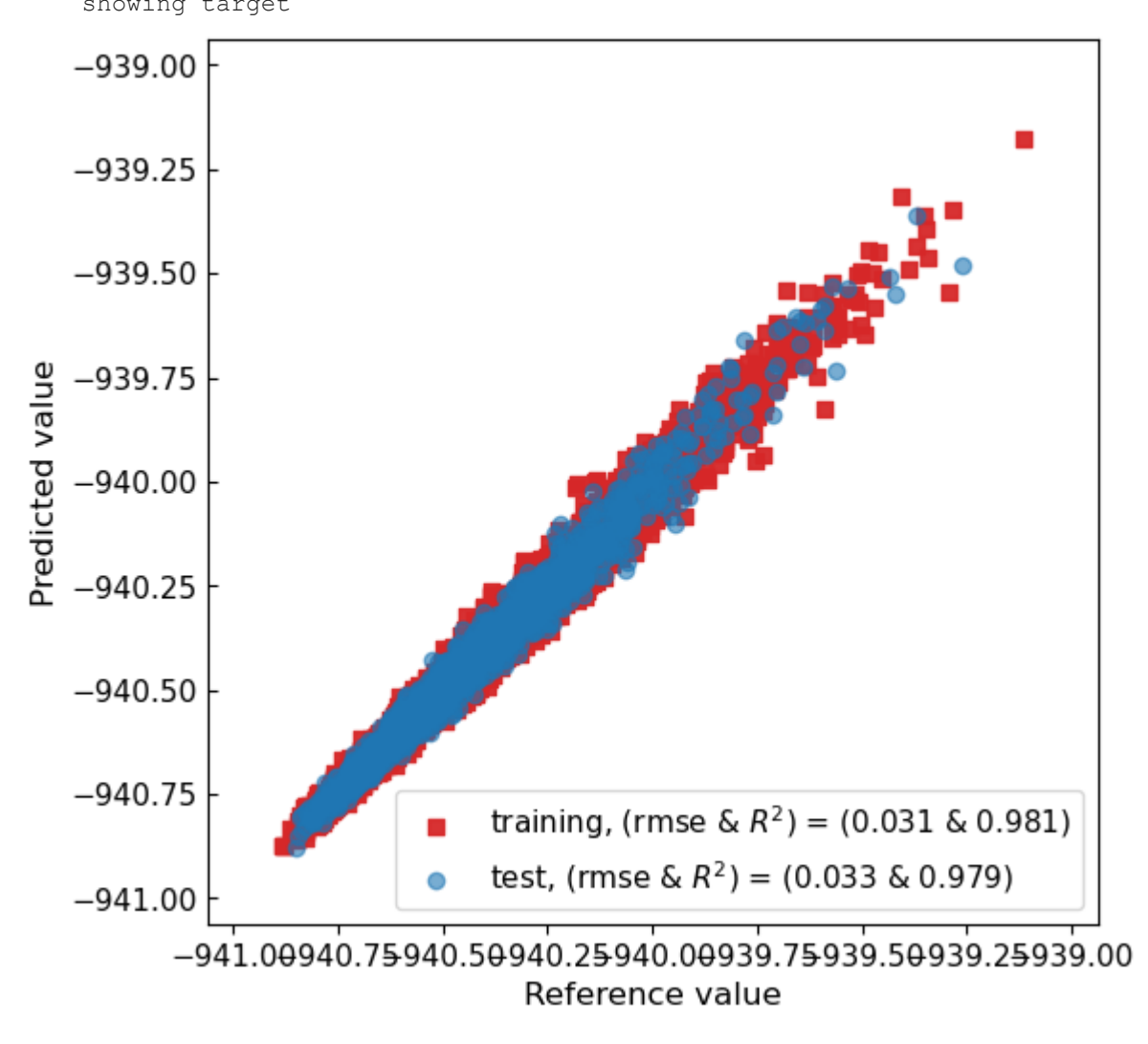
In [4]:
```
# data parameters for learning

id_col=['id']             # column for data ID
y_cols=['target']         # columns for (one or more) target properties
comment_cols=[]           # comment columns, anything not counted into ID, fingerprints, and target
n_trains=0.8              # 80% for training, 20% for validating
sampling='random'         # method for train/test spliting
x_scaling='minmax'        # method for x scaling
y_scaling='minmax'        # method for y scaling

# Dict of data parameters
data_params_pcm={'data_file':'fp_pcm.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_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}
```

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

# Model parameters
layers=[8,8,8]                 # list of nodes in hidden layers
epochs=200                    # 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

# Dict of model parameters
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}

# PCM
model=FCNN(data_params=data_params_pcm,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                         [8, 8, 8]
   activ_funct                    selu
   epochs                         200
   optimizer                      nadam
   nfold_cv                       5
 Reading data ...
   data file                      fp_pcm.csv
   data size                      9999
   training size                  7999 (80.0 %)
   test size                      2000 (20.0 %)
   x dimensionality               30
   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 0.068174 0.072319 0.072319
   cv,rmse_train,rmse_test,rmse_opt: 1 0.064059 0.072494 0.072319
   cv,rmse_train,rmse_test,rmse_opt: 2 0.064114 0.063432 0.063432
   cv,rmse_train,rmse_test,rmse_opt: 3 0.062374 0.064459 0.063432
   cv,rmse_train,rmse_test,rmse_opt: 4 0.062188 0.065128 0.063432
   Optimal ncv:  2 ; optimal NET saved
 FCNN trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           0.113256
   Unscaling y: minmax
      rmse test         target           0.113944
 Predictions made & saved in "training.csv" & "test.csv"

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



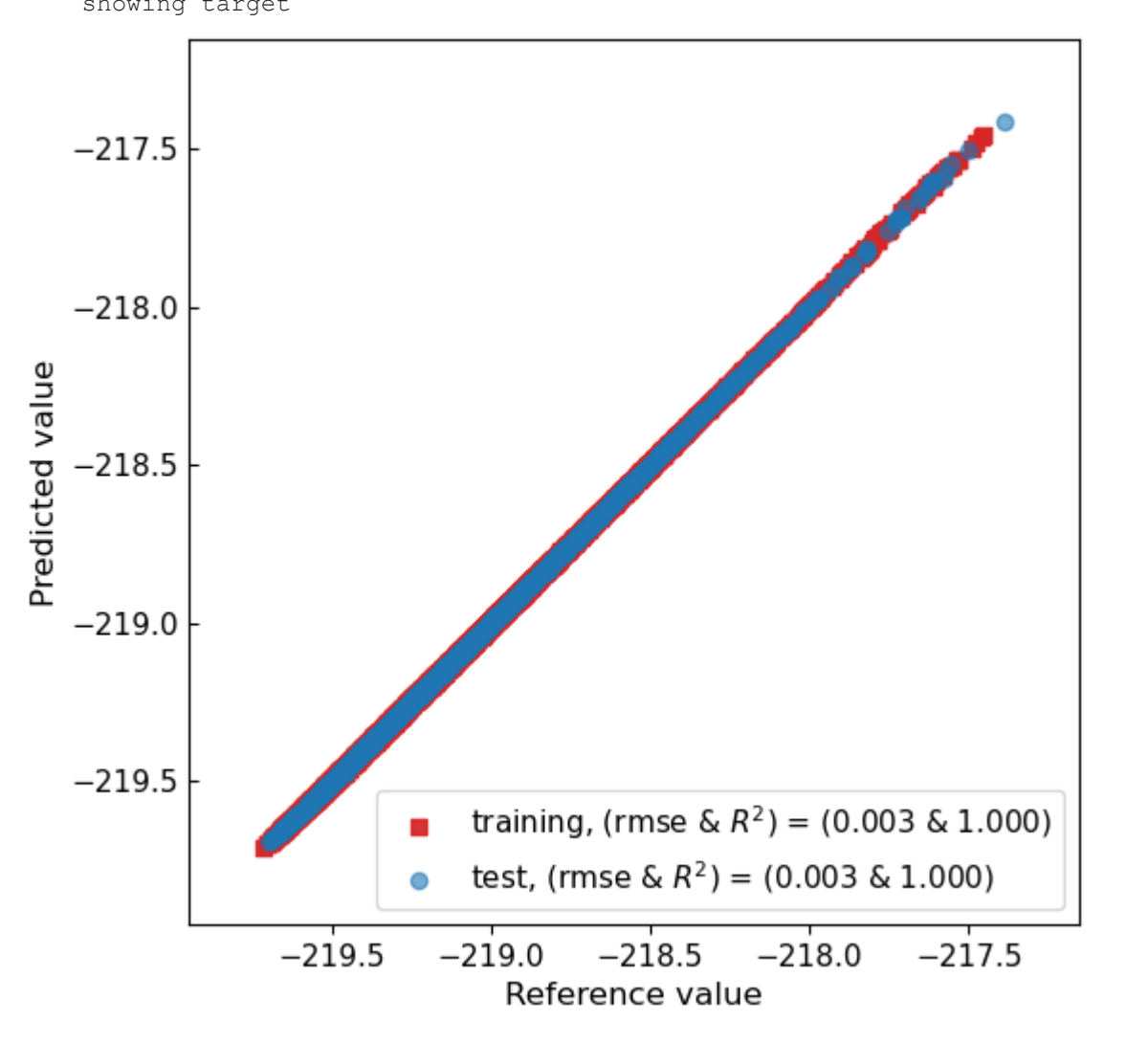

```
 Learning fingerprinted/featured data
   algorithm                      fully connected NeuralNet w/ TensorFlow
   layers                         [8, 8, 8]
   activ_funct                    selu
   epochs                         200
   optimizer                      nadam
   nfold_cv                       5
 Reading data ...
   data file                      fp_soap.csv
   data size                      9999
   training size                  7999 (80.0 %)
   test size                      2000 (20.0 %)
   x dimensionality               1050
   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 0.024478 0.025270 0.025270
   cv,rmse_train,rmse_test,rmse_opt: 1 0.019971 0.021035 0.021035
   cv,rmse_train,rmse_test,rmse_opt: 2 0.018775 0.019346 0.019346
   cv,rmse_train,rmse_test,rmse_opt: 3 0.017142 0.017984 0.017984
   cv,rmse_train,rmse_test,rmse_opt: 4 0.019387 0.020291 0.017984
   Optimal ncv:  3 ; optimal NET saved
 FCNN trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           0.030649
   Unscaling y: minmax
      rmse test         target           0.032979
 Predictions made & saved in "training.csv" & "test.csv"

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



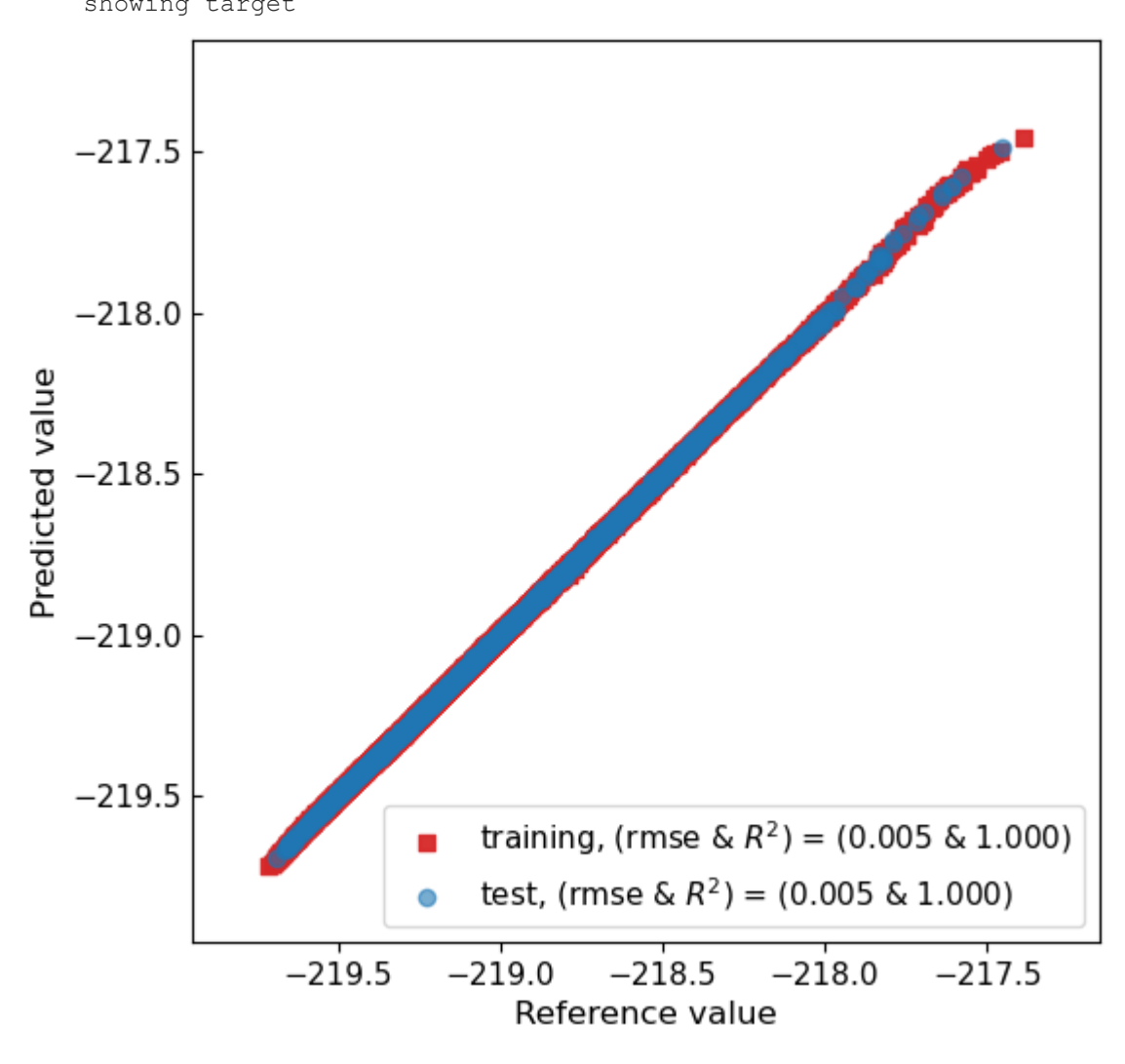
4. The same flowwork with the CH_4 dataset

In [6]:
```
# Load data
data=Datasets(dataset_name='molecs_CH4_10k')
data.load_dataset()
print (pd.read_csv('molecs_CH4_10k/summary.csv'))

# Fingerprint
from matsml.fingerprint import Fingerprint
summary=os.path.join(os.getcwd(),'molecs_CH4_10k/summary.csv')
data_loc=os.path.join(os.getcwd(),'molecs_CH4_10k/')
n_atoms_max=6                          # max number of atoms in all of the structures to be fingerprinted
fp_type='pcm_molecs'                   # projected Coulomb matrix for molecules
fp_dim=100                             # intended fingerprint dimensionality; the final number can be smaller
verbosity=0                            # verbosity, 0 or 1
species=['C','H']                      # All the spacies in the datasets, used for SOAP

# PCM
data_params_pcm={'fp_type':'pcm_molecs','summary':summary,'data_loc':data_loc,
    'n_atoms_max':n_atoms_max,'fp_file':'fp_CH4_pcm.csv','fp_dim':fp_dim,
    'species':species,'verbosity':verbosity}

fp_pcm=Fingerprint(data_params_pcm)
fp_pcm.get_fingerprint()

# SOAP
data_params_soap={'fp_type':'soap_molecs','summary':summary,'data_loc':data_loc,
    'species':species,'n_atoms_max':n_atoms_max,'fp_file':'fp_CH4_soap.csv',
    'fp_dim':fp_dim,'verbosity':verbosity}

fp_soap=Fingerprint(data_params_soap)
fp_soap.get_fingerprint()


# Data params
id_col=['id']             # column for data ID
y_cols=['target']         # columns for (one or more) target properties
comment_cols=[]           # comment columns, anything not counted into ID, fingerprints, and target
n_trains=0.8              # 80% for training, 20% for validating
sampling='random'         # method for train/test spliting
x_scaling='minmax'        # method for x scaling
y_scaling='minmax'        # method for y scaling

# Dict of data parameters
data_params_CH4_pcm={'data_file':'fp_CH4_pcm.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_CH4_soap={'data_file':'fp_CH4_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}


# Models with FCNN
from matsml.models import FCNN

# Model parameters
layers=[4,4]                   # list of nodes in hidden layers
epochs=200                    # 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='tanh'             # Options: "tanh", "relu", and more
optimizer='nadam'              # options: "Nadam", "Adam", and more

# Dict of model parameters
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}

# PCM
model=FCNN(data_params=data_params_CH4_pcm,model_params=model_params)
model.train()
model.plot(pdf_output=False)

#SOAP
model=FCNN(data_params=data_params_CH4_soap,model_params=model_params)
model.train()
model.plot(pdf_output=False)
```

```
 Load requested dataset(s)
   Data saved in molecs_CH4_10k
          file_name   target
0     CH4-00001.xyz -219.537
1     CH4-00002.xyz -219.117
2     CH4-00003.xyz -219.402
3     CH4-00004.xyz -219.155
4     CH4-00005.xyz -219.180
...             ...      ...
9995  CH4-09996.xyz -219.359
9996  CH4-09997.xyz -219.342
9997  CH4-09998.xyz -218.069
9998  CH4-09999.xyz -219.161
9999  CH4-10000.xyz -219.128

[10000 rows x 2 columns]
 Atomic structure fingerprinting
   summary                        /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH4_10k/summary.csv
   data_loc                       /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH4_10k/
   species                        ['C', 'H']
   fp_type                        pcm_molecs
   fp_file                        fp_CH4_pcm.csv
   fp_dim                         100
   n_atoms_max                    6
   verbosity                      0
 Read input
   num_structs                    10000
 Computing Coulomb matrix
   [==================================================] 100%
 Projecting Coulomb matrix to create fingerprints
   [==================================================] 100%
 Done fingerprinting, results saved in fp_CH4_pcm.csv
 Atomic structure fingerprinting
   summary                        /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH4_10k/summary.csv
   data_loc                       /home/huan/work/matsml/examples/ex1_pcm-molecs/molecs_CH4_10k/
   species                        ['C', 'H']
   fp_type                        soap_molecs
   fp_file                        fp_CH4_soap.csv
   fp_dim                         100
   n_atoms_max                    6
   verbosity                      0
 Read input
   num_structs                    10000
 Computing SOAP fingerprint
   [==================================================] 100%
 Done fingerprinting, results saved in fp_CH4_soap.csv

 Learning fingerprinted/featured data
   algorithm                      fully connected NeuralNet w/ TensorFlow
   layers                         [4, 4]
   activ_funct                    tanh
   epochs                         200
   optimizer                      nadam
   nfold_cv                       5
 Reading data ...
   data file                      fp_CH4_pcm.csv
   data size                      10000
   training size                  8000 (80.0 %)
   test size                      2000 (20.0 %)
   x dimensionality               36
   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 0.001728 0.001792 0.001792
   cv,rmse_train,rmse_test,rmse_opt: 1 0.001823 0.001871 0.001792
   cv,rmse_train,rmse_test,rmse_opt: 2 0.002435 0.002473 0.001792
   cv,rmse_train,rmse_test,rmse_opt: 3 0.001406 0.001354 0.001354
   cv,rmse_train,rmse_test,rmse_opt: 4 0.001378 0.001405 0.001354
   Optimal ncv:  3 ; optimal NET saved
 FCNN trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           0.003258
   Unscaling y: minmax
      rmse test         target           0.003258
 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                    tanh
   epochs                         200
   optimizer                      nadam
   nfold_cv                       5
 Reading data ...
   data file                      fp_CH4_soap.csv
   data size                      10000
   training size                  8000 (80.0 %)
   test size                      2000 (20.0 %)
   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 0.002481 0.002652 0.002652
   cv,rmse_train,rmse_test,rmse_opt: 1 0.002453 0.002506 0.002506
   cv,rmse_train,rmse_test,rmse_opt: 2 0.002143 0.003453 0.002506
   cv,rmse_train,rmse_test,rmse_opt: 3 0.002029 0.002155 0.002155
   cv,rmse_train,rmse_test,rmse_opt: 4 0.004519 0.004522 0.002155
   Optimal ncv:  3 ; optimal NET saved
 FCNN trained, now make predictions & invert scaling
   Unscaling y: minmax
      rmse training     target           0.004796
   Unscaling y: minmax
      rmse test         target           0.004675
 Predictions made & saved in "training.csv" & "test.csv"

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



In [ ]: