Example 2: Fingerpring molecules data and learning 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'
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 1.0.0
  *****
  Load requested dataset(s)
    Data saved in molecs_CH3NHOH
             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/summary.csv')
data_loc=os.path.join(os.getcwd(),'molecs_CH3NHOH/')
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/ex2_molecs/molecs_CH3NHOH/summary.csv
    data_loc                       /home/huan/work/matsml_examples/ex2_molecs/molecs_CH3NHOH/
    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/ex2_molecs/molecs_CH3NHOH/summary.csv
    data_loc                       /home/huan/work/matsml_examples/ex2_molecs/molecs_CH3NHOH/
    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_pcm',ds2='fp_molecs_CH3NHOH_soap')
data.load_dataset()

print (os.path.isfile('fp_molecs_CH3NHOH_pcm.csv.gz'))
print (os.path.isfile('fp_molecs_CH3NHOH_soap.csv.gz'))
```

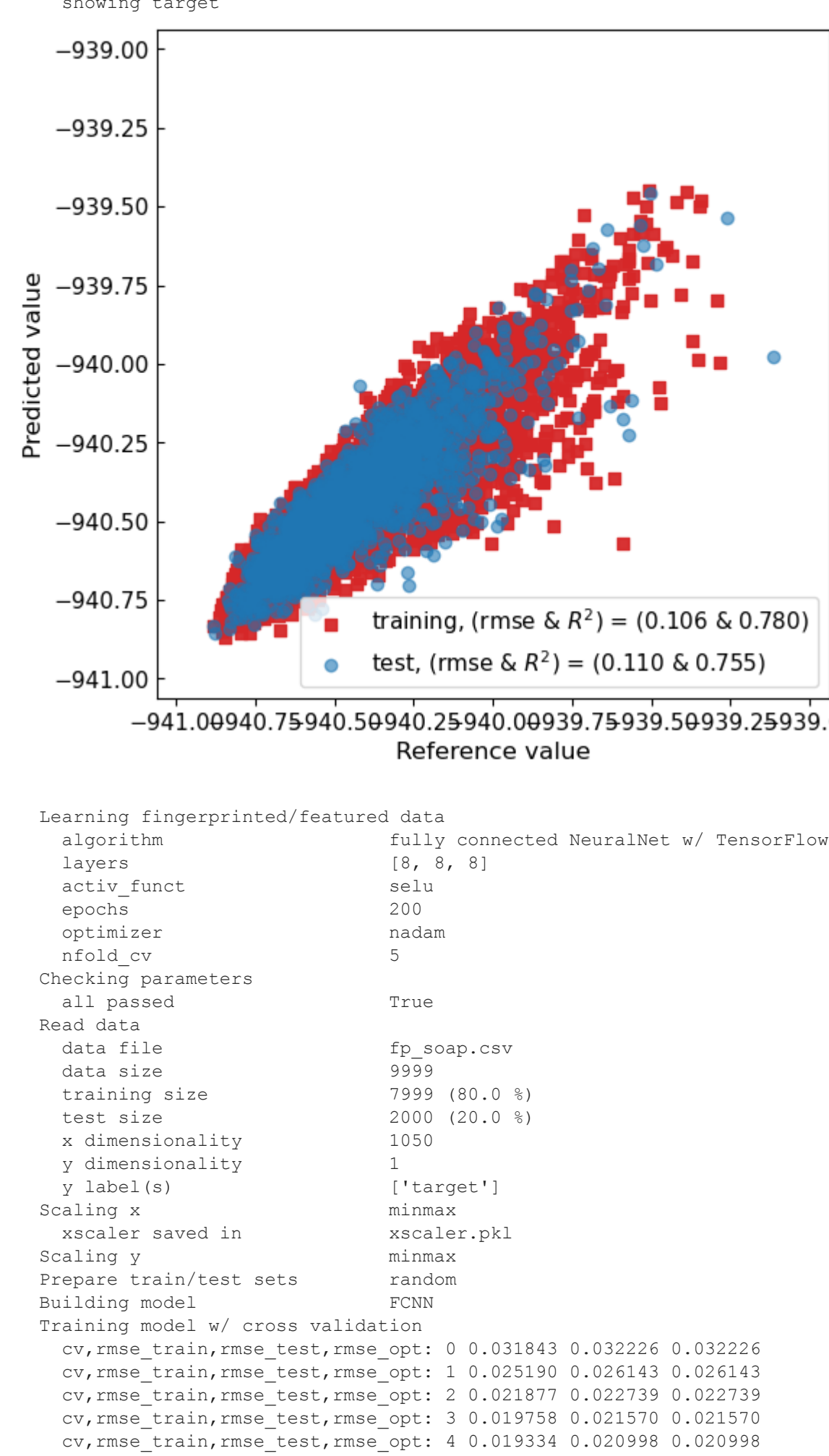
```
  Load requested dataset(s)
    Data saved in fp_molecs_CH3NHOH_pcm.csv.gz
    Data saved in fp_molecs_CH3NHOH_soap.csv.gz
True
True
```

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
  Checking parameters
    all passed                     True
  Read 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 0.067107 0.076397 0.076397
    cv,rmse_train,rmse_test,rmse_opt: 1 0.061339 0.064787 0.064787
    cv,rmse_train,rmse_test,rmse_opt: 2 0.059690 0.060570 0.060570
    cv,rmse_train,rmse_test,rmse_opt: 3 0.058808 0.061223 0.060570
    cv,rmse_train,rmse_test,rmse_opt: 4 0.059099 0.062423 0.060570
    Optimal ncv:  2 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           0.105978
    unscaling y: minmax
       rmse test         target           0.109507
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.106 & 0.780)
    test, (rmse & R2) = (0.110 & 0.755)
    showing target
```

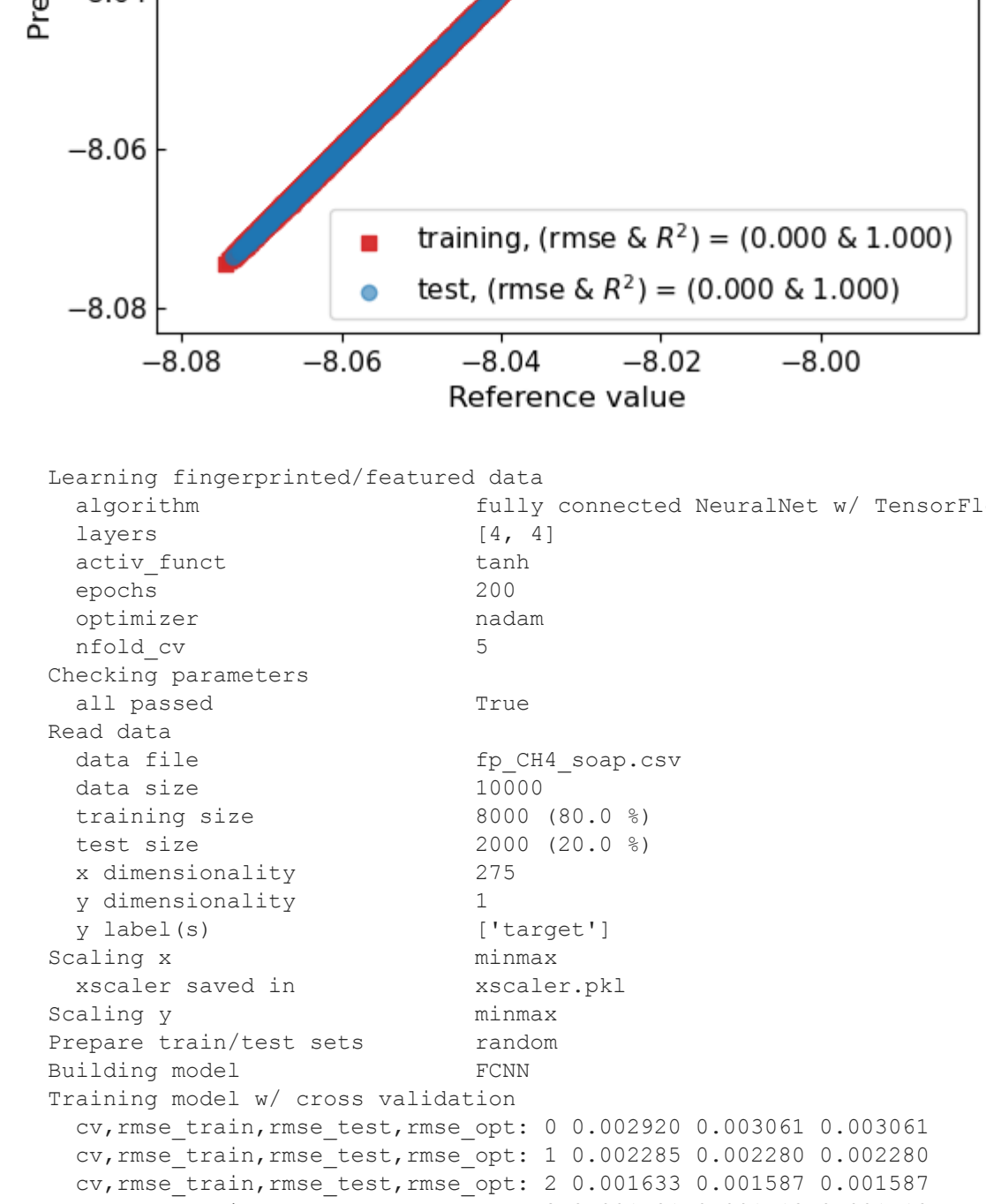



```
  Learning fingerprinted/featured data
    algorithm                      fully connected NeuralNet w/ TensorFlow
    layers                         [8, 8, 8]
    activ_funct                    selu
    epochs                         200
    optimizer                      nadam
    nfold_cv                       5
  Checking parameters
    all passed                     True
  Read 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 0.031843 0.032226 0.032226
    cv,rmse_train,rmse_test,rmse_opt: 1 0.025190 0.026143 0.026143
    cv,rmse_train,rmse_test,rmse_opt: 2 0.021877 0.022739 0.022739
    cv,rmse_train,rmse_test,rmse_opt: 3 0.019758 0.021570 0.021570
    cv,rmse_train,rmse_test,rmse_opt: 4 0.019334 0.020998 0.020998
    Optimal ncv:  4 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           0.034835
    unscaling y: minmax
       rmse test         target           0.037249
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.035 & 0.976)
    test, (rmse & R2) = (0.037 & 0.972)
    showing target
```

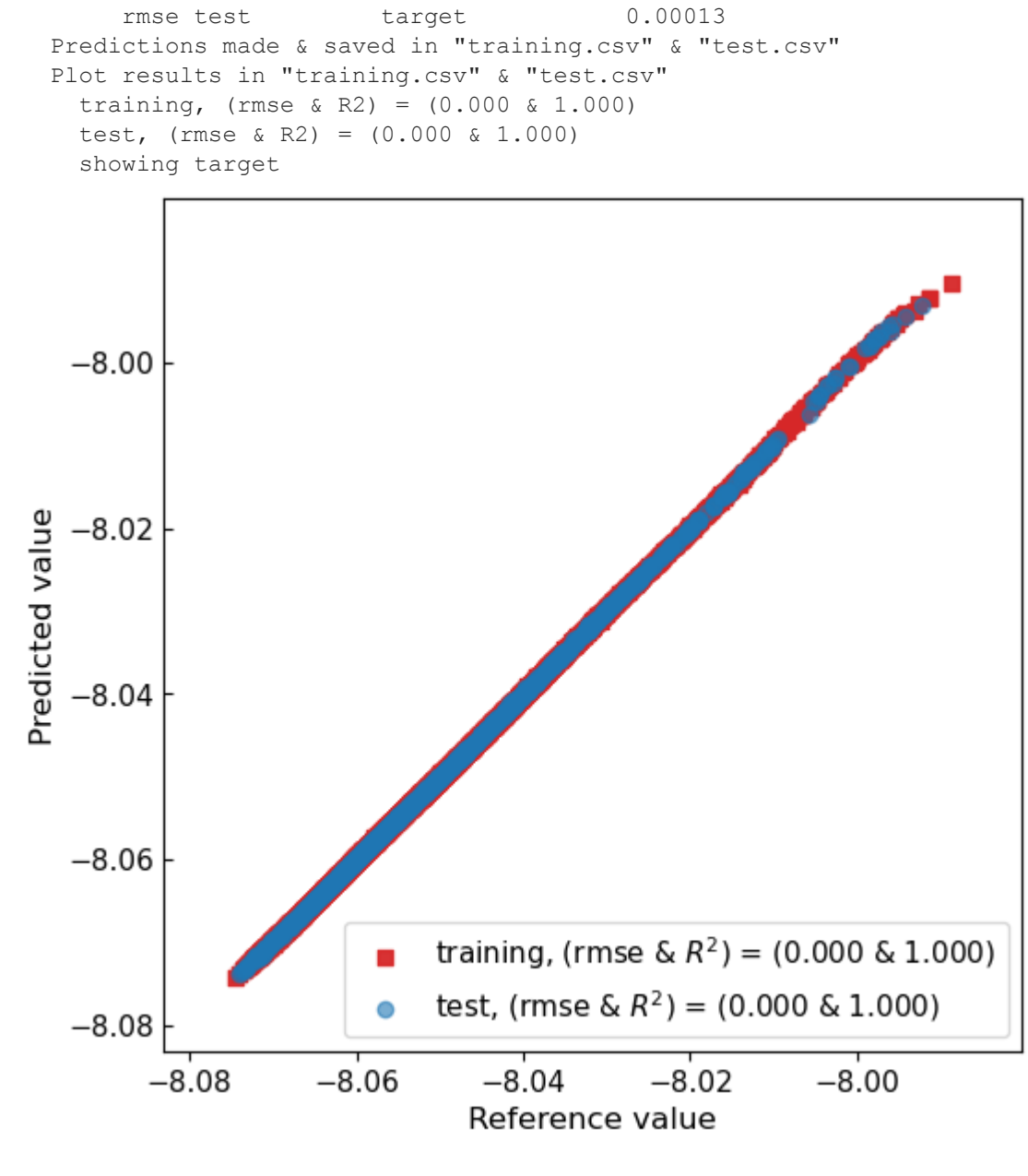
4. The same flowwork with the CH_4 dataset

In [6]:
```
# Load data
data=Datasets(dataset_name='molecs_CH4')
data.load_dataset()
print (pd.read_csv('molecs_CH4/summary.csv'))

# Fingerprint
from matsml.fingerprint import Fingerprint
summary=os.path.join(os.getcwd(),'molecs_CH4/summary.csv')
data_loc=os.path.join(os.getcwd(),'molecs_CH4/')
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
         file_name    target
0     CH4-00001.xyz -8.067843
1     CH4-00002.xyz -8.052410
2     CH4-00003.xyz -8.062879
3     CH4-00004.xyz -8.053809
4     CH4-00005.xyz -8.054724
...             ...       ...
9995  CH4-09996.xyz -8.061287
9996  CH4-09997.xyz -8.060672
9997  CH4-09998.xyz -8.013882
9998  CH4-09999.xyz -8.054027
9999  CH4-10000.xyz -8.052808

[10000 rows x 2 columns]
  Atomic structure fingerprinting
    summary                        /home/huan/work/matsml_examples/ex2_molecs/molecs_CH4/summary.csv
    data_loc                       /home/huan/work/matsml_examples/ex2_molecs/molecs_CH4/
    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/ex2_molecs/molecs_CH4/summary.csv
    data_loc                       /home/huan/work/matsml_examples/ex2_molecs/molecs_CH4/
    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
  Checking parameters
    all passed                     True
  Read 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 0.002489 0.002526 0.002526
    cv,rmse_train,rmse_test,rmse_opt: 1 0.002041 0.002149 0.002149
    cv,rmse_train,rmse_test,rmse_opt: 2 0.001434 0.001373 0.001373
    cv,rmse_train,rmse_test,rmse_opt: 3 0.001359 0.001398 0.001373
    cv,rmse_train,rmse_test,rmse_opt: 4 0.001499 0.001505 0.001373
    Optimal ncv:  2 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           0.000122
    unscaling y: minmax
       rmse test         target           0.000125
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.000 & 1.000)
    test, (rmse & R2) = (0.000 & 1.000)
    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
  Checking parameters
    all passed                     True
  Read 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 0.002920 0.003061 0.003061
    cv,rmse_train,rmse_test,rmse_opt: 1 0.002285 0.002280 0.002280
    cv,rmse_train,rmse_test,rmse_opt: 2 0.001633 0.001587 0.001587
    cv,rmse_train,rmse_test,rmse_opt: 3 0.001481 0.001512 0.001512
    cv,rmse_train,rmse_test,rmse_opt: 4 0.001787 0.001774 0.001512
    Optimal ncv:  3 ; optimal NET saved
  FCNN trained, now make predictions & invert scaling
    unscaling y: minmax
       rmse training     target           0.000128
    unscaling y: minmax
       rmse test         target           0.00013
  Predictions made & saved in "training.csv" & "test.csv"
  Plot results in "training.csv" & "test.csv"
    training, (rmse & R2) = (0.000 & 1.000)
    test, (rmse & R2) = (0.000 & 1.000)
    showing target
```



In [ ]: