trainThermoNetNew

March 16, 2022

[219]:
```
import numpy as np
import torch
from torch.utils.data import DataLoader
from torch.optim import RMSprop, SGD
from torch.optim.lr_scheduler import ExponentialLR
from torch.nn import MSELoss
import matplotlib.pyplot as plt

from thermonet.net import ThermoNetNew
from thermonet.dataset import ThermoDatasetNew
from utils.plot import PlotHandler
```

[224]:
```
def epoch(net, dataloader, loss_func, optimizer, scheduler):
    epoch_losses = np.zeros([len(dataloader), ])

    for i, d in enumerate(dataloader):
        inp = d[:, [0, -2, -1]]
        targets = d[:, [1, 2, 3, 4]]

        # Forward pass
        predictions = net(inp.float())

        # Get the loss
        loss = loss_func(predictions, targets.float())

        # Backward pass
        net.zero_grad()
        loss.backward()
        optimizer.step()
        epoch_losses[i] = loss
    scheduler.step()

    mean_epoch_loss = epoch_losses.mean(axis=0)
    #print('Mean epoch loss: ', mean_epoch_loss)
    return mean_epoch_loss

def train(net, dataloader, optimizer, scheduler, loss_func, nr_epochs=500):
    losses = []
```

```
    best_loss = epoch(net, dataloader, loss_func, optimizer, scheduler)
    best_net = net

    ph = PlotHandler()

    for i in range(nr_epochs):
        #print('-----\nEpoch %i:\n' % i)
        loss = epoch(net, dataloader, loss_func, optimizer, scheduler)
        losses.append(loss)

        if loss < best_loss:
            best_net = net

        if i % 10 == 0:
            print(i, ': ', loss)
            print('lr: ', scheduler.get_last_lr())
            last_losses = np.array(losses[-50:])
            last_losses_std, last_losses_mean = last_losses.std(), last_losses.
↪mean()
            last_loss_diffs = np.diff(last_losses)
            print(np.mean(last_loss_diffs))
            print(last_losses_std/np.mean(last_loss_diffs), last_losses_std,␣
↪last_losses_mean)
            print()

        if i % 250 == 0:
            ph.properties_temp_modified_new(best_net, ['Fe'], 'BCC_A2',␣
↪start_temp=200, end_temp=2000)
            plt.plot(losses)

    return losses, net
```

[236]:
```
# Hyperparameters
nr_epochs = 2500
lr = 0.005 # 0.000025
batch_size = 256
hidden_size = 128
hidden_layers = 8
```

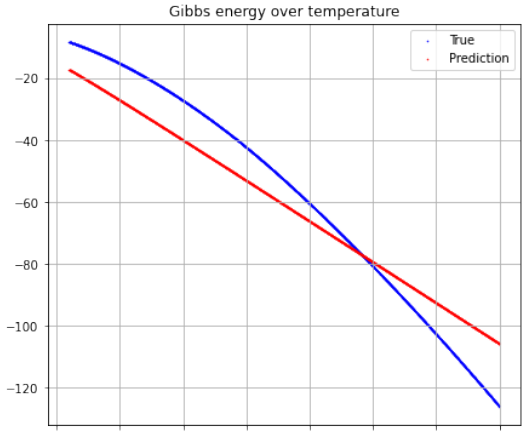
[237]:
```
# Network
net = ThermoNetNew(hidden_size_linear=hidden_size, hidden_layers=hidden_layers)

# Optimizer
optimizer = RMSprop(net.parameters(), lr=lr)
scheduler = ExponentialLR(optimizer, gamma=0.995)
```

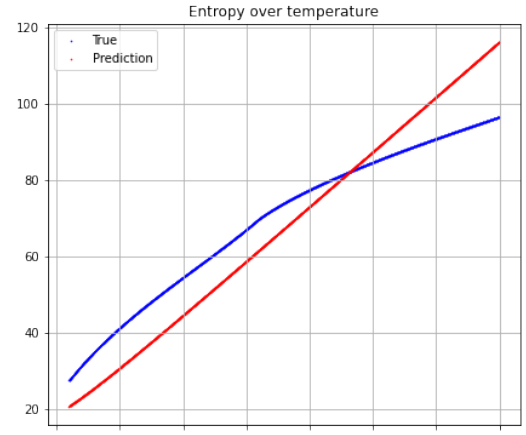
```
# Loss function
loss_func = MSELoss()
```

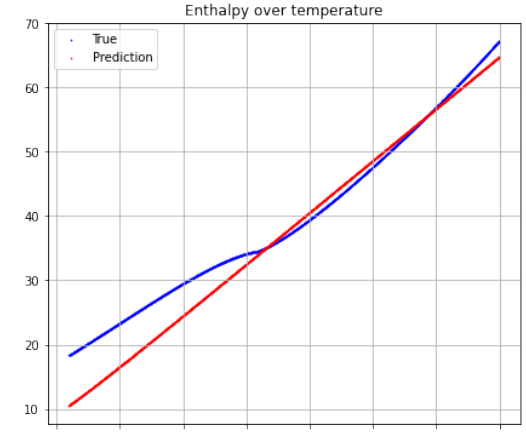
[238]:
```
# Dataset
start_temp, end_temp = 200, 2000
step = 1
dataset = ThermoDatasetNew(['Fe'], start_temp=start_temp, end_temp=end_temp,␣
 ↪step=step)
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=True)
```

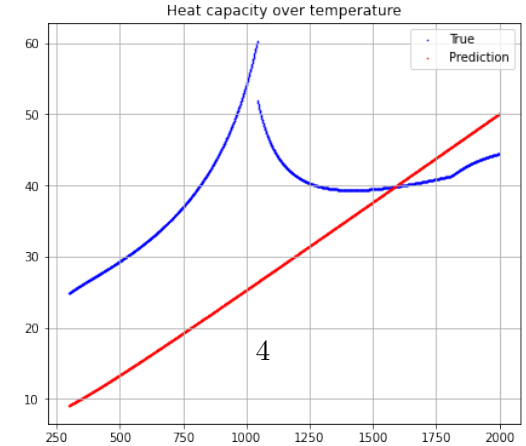
[239]:
```
losses, best_net = train(net, dataloader, optimizer=optimizer,␣
 ↪scheduler=scheduler, loss_func=loss_func, nr_epochs=nr_epochs)
```

```
0 :  402.19446029663084
lr:  [0.0049501250000000005]
nan
nan 0.0 402.19446029663084
```


Gibbs energy over temperature
True
Prediction
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
120
100
80
60
40
20

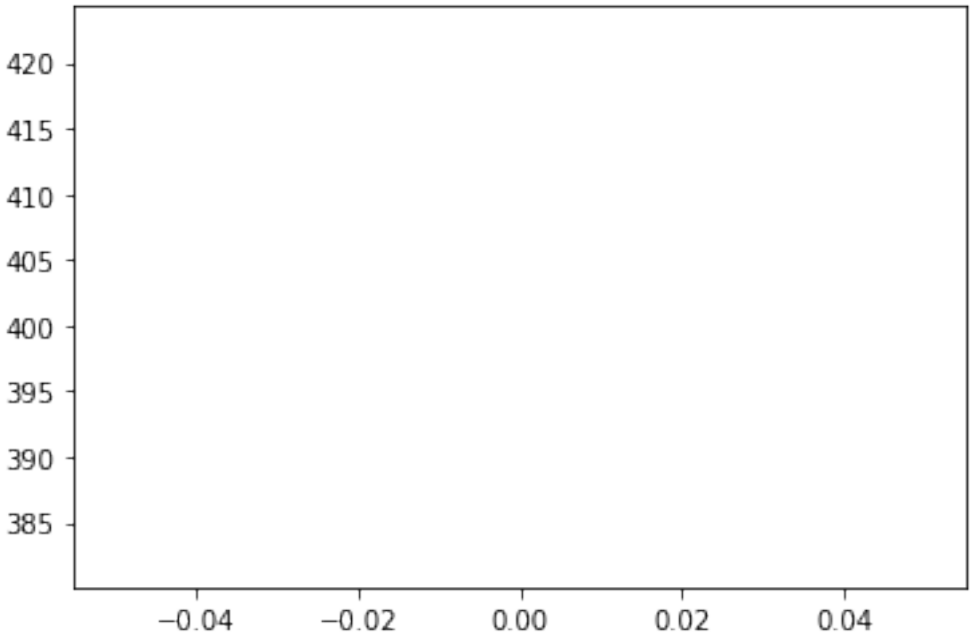

Enthalpy over temperature
True
Prediction
70
60
50
40
30
20
10

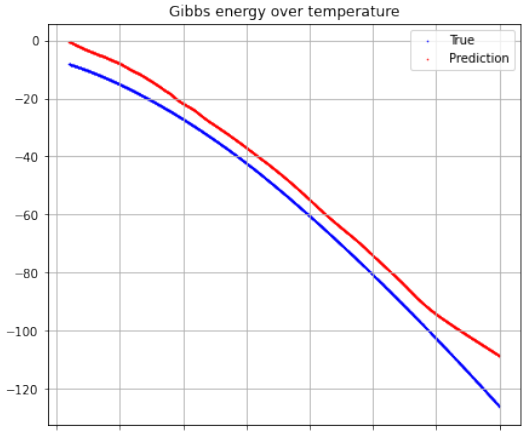

Heat capacity over temperature
True
Prediction
60
50
40
30
20
10
250
500
750
1000
1250
1500
1750
2000

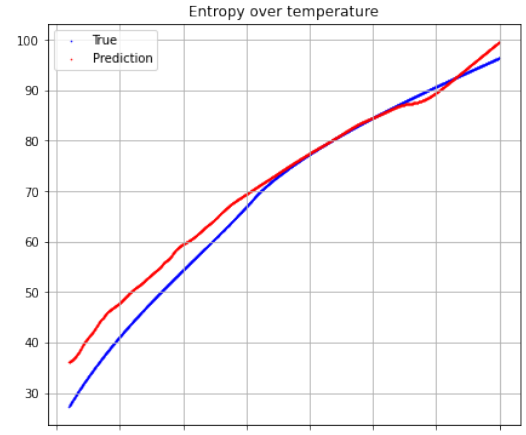
```
10 :  108.820423634847
lr:  [0.0047081140345718794]
-29.337403666178382
-3.1265329424430472 91.72435900805614 155.06582195397576

20 :  118.85357666015625
lr:  [0.004477934953669392]
-14.16704418182373
-4.933282941449753 69.89003739295597 134.7396277291434

30 :  110.63458150227865
lr:  [0.004259009298001735]
-9.718662626875766
-4561427.287197333 44330972.90129603 8093837.367448705

40 :  114.4238047281901
lr:  [0.0040507868890773645]
-7.194266389310355
-5379822.752793409 38703878.010868736 6119758.318061066

50 :  106.98911666870117
lr:  [0.0038527444465594088]
0.04394747708119506
799284551.0212973 35126539.48736175 5018801.168489487

60 :  104.4120699564616
lr:  [0.003664384273218397]
-0.026804855486162474
-1310454374.8559203 35126540.13922233 5018796.605963353

70 :  82.34311498006186
lr:  [0.003485233004177472]
-5120499.868683012
-6.8599826782141315 35126540.4029632 5018794.760003591

80 :  119.63494135538737
lr:  [0.0033148404173068496]
0.2003864002876441
20452.261575523877 4098.35507486053 694.1846575368247

90 :  125.32510096232096
lr:  [0.0031527783017779305]
0.3119762965611049
13136.783929650248 4098.365199095723 694.1357814280194
```

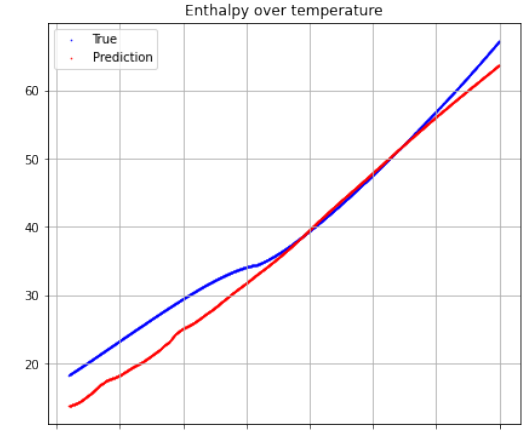
```
100 :  111.49432678222657
lr:  [0.0029986393819336618]
-0.13172689424894957
-20472.21531419049 2696.7413417340963 492.4009976806641

110 :  122.49540506998697
lr:  [0.002852036293770727]
0.20340638971652145
13256.326759740394 2696.4215671013067 494.949673634847

120 :  102.75962626139322
lr:  [0.0027126006114613927]
-0.5275826253046716
-5110.260190297115 2696.084487186902 497.31411435190836

130 :  90.40528996785481
lr:  [0.0025799819214685775]
-0.12502958855655952
-21565.81643414126 2696.3651556469713 495.2914328511556

140 :  65.18328526814778
lr:  [0.002453846941927312]
-0.7969216742482487
-3384.248475791555 2696.9809613998896 491.1812508824667

150 :  66.97488085428874
lr:  [0.002333878685079522]
-0.7482816605340867
-108.07193813400835 80.86824932405285 110.98112246576946

160 :  55.70129674275716
lr:  [0.0022197756606572683]
-1.4208873878530919
-57.08391080831335 81.10980891686323 100.49819825871786

170 :  47.068220647176105
lr:  [0.0021112511182124795]
-0.9015669089596287
-91.12653911491296 82.15667219402077 88.86684828058878

180 :  45.84127082824707
lr:  [0.0020080323264890774]
-1.3411146202865938
-62.111705748261265 83.29891666993205 78.62940737406413

190 :  39.76497662862142
lr:  [0.0019098598880265135]
-1.3375021668518459
```

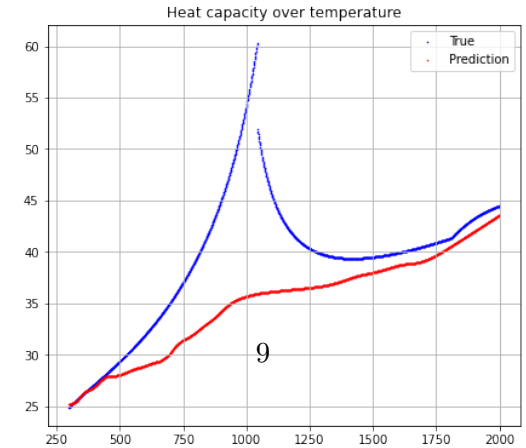
```
-81.57134488796326 109.1018505406701 84.89401067479452

200 :  44.826606623331706
lr:  [0.0018164870872722418]
-0.5359394384890195
-140.32433922480163 75.20534757048287 69.09981006749472

210 :  39.44840799967448
lr:  [0.0017276792705648916]
-0.5487428185080168
-138.35564885755522 75.92166871060033 64.30134247334799

220 :  30.01831029256185
lr:  [0.0016432132564299833]
-0.35510702587309406
-216.0139740831129 76.70807988368185 60.309242829640695

230 :  25.98142458597819
lr:  [0.001562876774706207]
-9.20520045611323
-8.408503842981139 77.40196341063982 57.294417836507165

240 :  27.351262664794923
lr:  [0.001486467933092745]
-0.29092196120696795
-39.545816460545495 11.504746482232692 38.63470184834798

250 :  29.676887702941894
lr:  [0.0014137947097770268]
-0.315230485046802
-23.79468460633586 7.500809969990926 34.656044300079344
```


420
415
410
405
400
395
390
385
−0.04
−0.02
0.00
0.02
0.04


Gibbs energy over temperature
True
Prediction
0
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
100
90
80
70
60
50
40
30

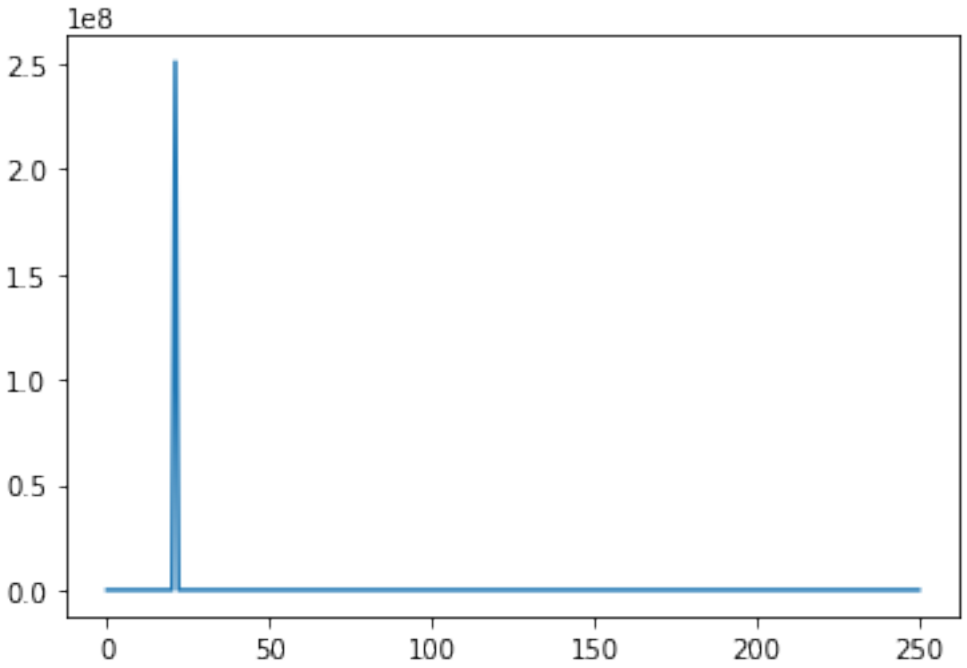

Enthalpy over temperature
True
Prediction
60
50
40
30
20

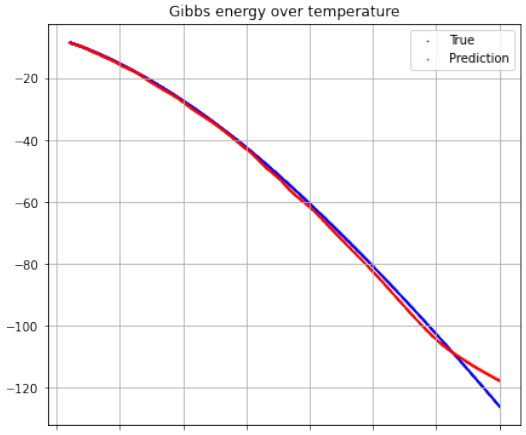

Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

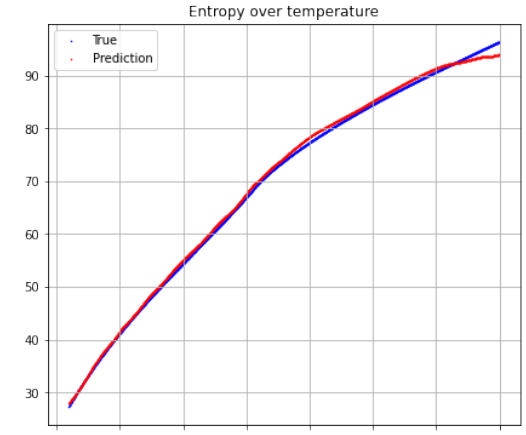
```
260 :  26.55934804280599
lr:  [0.0013446744708678 46]
-0.2821840610633903
-18.446736314124703 5.205374966485224 31.192514255523683

270 :  25.194944127400717
lr:  [0.0012789335114211096]
-0.3427779658311078
-13.068615437794065 4.479633415996062 28.91315288925171

280 :  24.280556265513102
lr:  [0.001216406618904779]
-0.18008289791288837
-19.270709979983263 3.470325298034205 27.02865652783712

290 :  22.29704844156901
lr:  [0.0011569366580059526]
-0.2303661969243263
-11.207934036214379 2.5819291393014208 25.59525926399231

300 :  20.49740924835205
lr:  [0.0011003741757366753]
-0.06778957211241435
-31.163300479257543 2.112546805099466 24.342902364730836

310 :  19.365006351470946
lr:  [0.0010465770258460752]
-0.16421891621180948
-12.898680991609412 2.1182074130039656 23.188348529179898

320 :  20.29968852996826
lr:  [0.00099541001159494]
-0.05974581711957248
-36.42775776539685 2.1764061535274863 22.06906722768148

330 :  18.24223937988281
lr:  [0.0009467445459949988]
-0.12109375648758043
-18.716232206566474 2.2664188651869708 20.879414628346762

340 :  16.272246424357096
lr:  [0.0009004583286590612]
-0.14201088859921407
-16.508949766959407 2.3444506262456937 19.518475668589275
```

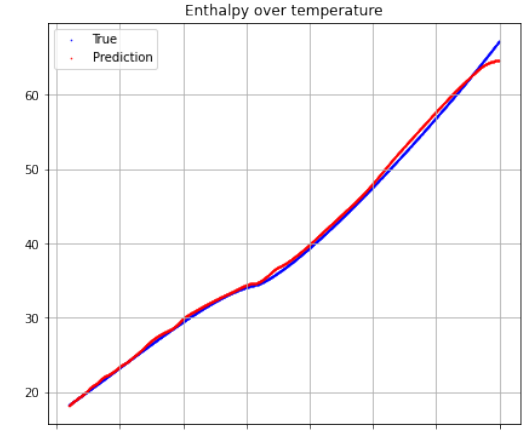
```
350 :  13.844119326273601
lr:  [0.0008564350384499106]
-0.16030923752557663
-16.439249883263663 2.6353636142784227 18.012640593528747

360 :  16.969230858484902
lr:  [0.0008145640411555528]
-0.07576227869306294
-36.216476047472455 2.7438427515892467 16.536684475898742

370 :  11.322080485026042
lr:  [0.000774740111456184]
-0.14362623837529398
-17.499768837961078 2.513425970633539 15.100198700269063

380 :  9.808874066670736
lr:  [0.0007368631684841578]
-0.15327578823582652
-15.899540385985292 2.437014585249253 13.629595552762348

390 :  6.709784905115764
lr:  [0.0007008380243123892]
-0.20949393518927956
-11.75201613642433 2.4619761068274464 12.317091055552163

400 :  10.759837627410889
lr:  [0.0006665741447391304]
-0.04193952424185617
-62.57923564992344 2.624543370576794 11.081858956972756

410 :  1.443538839618365
lr:  [0.0006339854217679446]
-0.23288123788071327
-12.689099928362024 2.9550532989090184 9.901314210792384

420 :  13.295627768834432
lr:  [0.0006029899572111071]
0.011684496224332033
282.5097593091154 3.30098421598431 8.947874459326266

430 :  8.779482320944469
lr:  [0.0005735098568726064]
-0.019259547781781898
-168.4787795279318 3.2448251045345007 8.259924062391123

440 :  9.531562546888987
lr:  [0.0005454710347935108]
0.01340487303377021
```

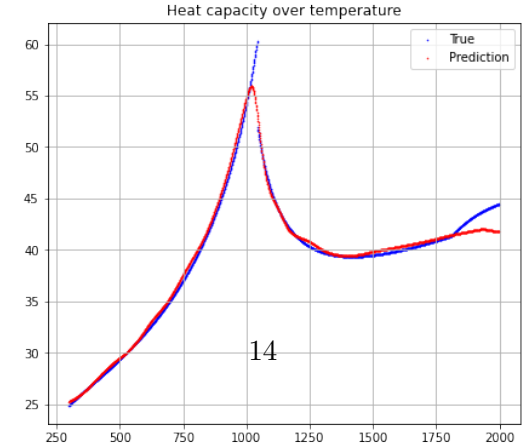
```
258.23425229221834 3.4615973649477705 7.287620421985785

450 :  1.1128710707028706
lr:  [0.00051880302706775 57]
-0.1427974012433265
-27.080081631008085 3.8669652823650966 6.437408661544323

460 :  2.3242450137933095
lr:  [0.0004934388147604504]
-0.17909987544526837
-21.022167027720556 3.765067496254379 5.875306760152181

470 :  1.7158323307832082
lr:  [0.00046931465548368765]
-0.19898608099846618
-16.662153833713525 3.315536692364223 4.987742814203103

480 :  2.967610611518224
lr:  [0.000446369923206589]
-0.03675658901532491
-87.668626159798 3.222399661293857 4.159121151939034

490 :  1.1579375753800074
lr:  [0.00042454695589701544]
-0.09163883861635817
-34.76459848099352 3.185787429762256 3.8217701390484966

500 :  0.9170005261898041
lr:  [0.0004037909106120566]
-0.013128563944174434
-238.2605140477309 3.128018394047506 3.397684303154548
```


1e8
2.5
2.0
1.5
1.0
0.5
0.0
0
50
100
150
200
250


Gibbs energy over temperature
True
Prediction
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
90
80
70
60
50
40
30


Enthalpy over temperature
True
Prediction
60
50
40
30
20


Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

```
510 :  1.2814665536085765
lr:  [0.00038404962567312596]
-0.17023235908170944
-17.887513063220265 3.0450335468568808 2.956093535343806

520 :  4.010370841622352
lr:  [0.0003652734895792976]
0.06682465590384559
44.32197415136023 2.961800671643786 2.811849965922534

530 :  0.717447595546643
lr:  [0.00034741531632945347]
-0.12707413376695445
-22.627453377270644 2.875364037268815 2.468292429832121

540 :  0.6204685171445211
lr:  [0.0003304302268399139]
-0.0025533969305000107
-1017.4011323287431 2.597828928375448 2.099341849200427

550 :  0.6420670285820961
lr:  [0.00031427553615954513]
-0.005898763563762753
-413.71126332631064 2.440384926027499 2.1308316569005448

560 :  0.27792124127348267
lr:  [0.00029891064619890525]
-0.009275259399393733
-248.26943836250913 2.302763441754066 1.9323918180763722

570 :  6.005263300736745
lr:  [0.000284296943703849]
0.12035195446085366
18.188981235561833 2.1890794413516597 1.7101266693348685

580 :  0.6763814183572928
lr:  [0.000270397703217188]
-0.09830346105962384
-20.174597515374888 1.9832327612462393 1.5008658636485541

590 :  0.09178777324656645
lr:  [0.0002571779947845447]
-0.012601854081968853
-171.0140547523039 2.1550941639543657 1.5465038825273512
```

```
600 :  0.42000230252742765
lr:  [0.0002446045961724539]
-0.001078188652489438
-1749.2991773089393 1.8860745227836078 1.2728401659503579

610 :  0.3906961182753245
lr:  [0.00023264590937811005]
-0.011544775917213776
-151.3345008558994 1.7471229009247549 1.1354132700661819

620 :  0.3528879108528296
lr:  [0.0002212718812209424]
-0.017167558105421768
-91.35438575726673 1.5683317256729914 0.9941828935816885

630 :  0.2321213662624359
lr:  [0.0002104539278164573]
-0.16526489618684165
-9.752328398902455 1.6117175404246018 0.9985234778883557

640 :  0.45949785473446053
lr:  [0.00020016486274254485]
-0.0009108553520169186
-1282.6978752147772 1.1683522246601095 0.7610830796696245

650 :  0.23341731466352938
lr:  [0.00019037882871772517]
-0.0004345836409298027
-2379.4915448177967 1.034088099108599 0.6831474026789267

660 :  0.13713627535228928
lr:  [0.00018107123261963643]
-0.08830692761951468
-11.192225469371579 0.9883510444250848 0.6166669323326399

670 :  0.08150605885311961
lr:  [0.0001722186836804605]
-0.006717427056536196 5
-122.83424520719436 0.825130082224009 0.5204605838687469

680 :  0.15301464330404996
lr:  [0.0001637989347039663]
-0.0670584925418707
-11.364410320880868 0.762080224745548 0.4681378303909054

690 :  2.444952892512083
lr:  [0.00015579082615644384]
0.04757033309892934
```

```
14.620004178205555 0.695478468664977 0.42503448071982725

700 :  0.15844037663191557
lr:  [0.00014817423299102564]
-0.002592863772241858
-233.72364853720842 0.6060135810083165 0.353145302512683

710 :  0.15507892022530237
lr:  [0.00014093001407176005]
-0.0009952118962394758
-513.3546459984301 0.5108966506874425 0.3045484586820627

720 :  0.16604876319567363
lr:  [0.00013403996407033 48]
-0.0012836942892698944
-341.8804761286752 0.4388700148192528 0.25173661297683914

730 :  0.3498848809239765
lr:  [0.0001274867677145635]
0.002032281630070654
191.36051193447906 0.388898453125358 0.2256279043822239

740 :  0.10567658636718988
lr:  [0.00012125395627365804]
0.0006207823328876588
364.34461311512683 0.22617869890465991 0.16509384514872605

750 :  0.03236707175771395
lr:  [0.00011532586617092 99]
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```

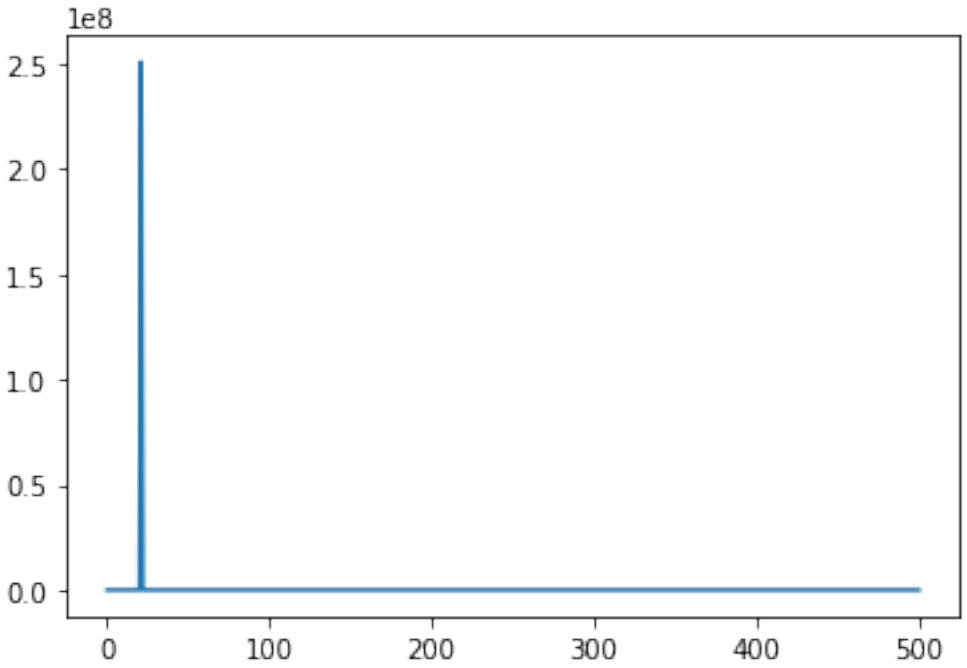
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2.5
2.0
1.5
1.0
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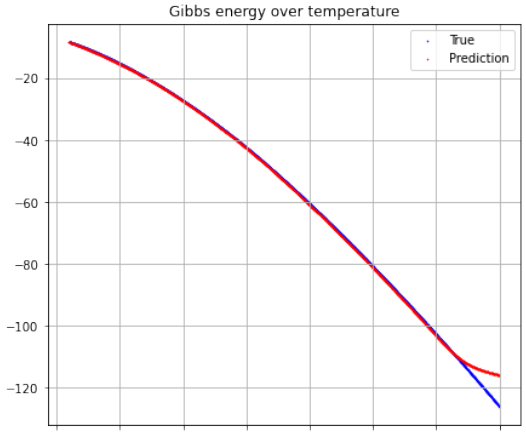
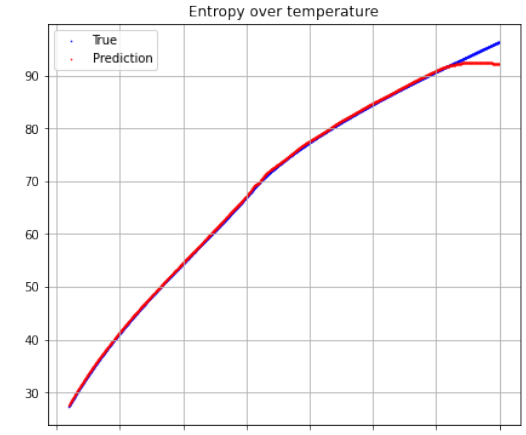
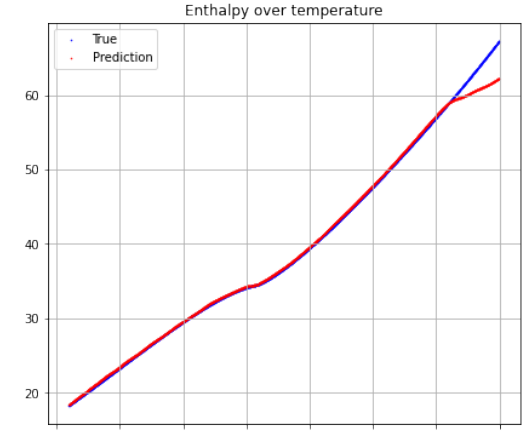
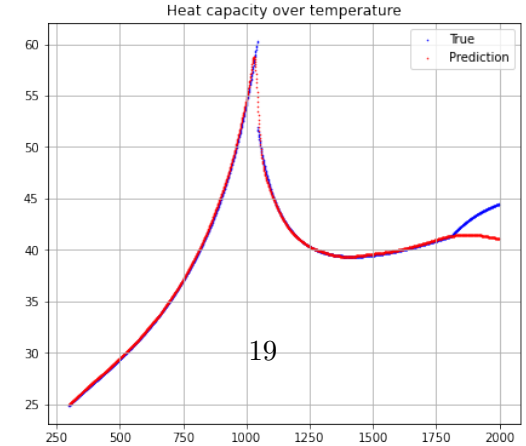
0.0
0
100
200
300
400
500


Gibbs energy over temperature
True
Prediction
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
90
80
70
60
50
40
30


Enthalpy over temperature
True
Prediction
60
50
40
30
20


Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

```
760 :  0.09114159618814786
lr:  [0.00010968759961991128]
-2.1817746135047676e-05
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770 :  0.05849488607297341
lr:  [0.00010432498718497115]
-6.032377278724097e-05
-2872.6497620513187 0.17328907154330558 0.1281654414992469

780 :  0.4915197292032341
lr:  [9.922455217233788e-05]
0.009755793675070712
16.060405969862867 0.15668200697985604 0.11169739019700017

790 :  0.05828011160095533
lr:  [9.437347676204006e-05]
0.0005617630484254101
279.81186985136065 0.15718796899331447 0.10433722804983457

800 :  0.018825399146104854
lr:  [8.975956979565241e-05]
-0.0020305818260400277
-49.999639815038314 0.10152835991696417 0.08294259626325219

810 :  0.04730071130519112
lr:  [8.537123613889452e-05]
0.0003792097614634563
284.21911049386387 0.10777866109373385 0.08128922909117925

820 :  0.30596701400354503
lr:  [8.11974475420882e-05]
0.004541266071578472
17.90368389270931 0.08130539221822677 0.0729713794932856

830 :  0.028833089768886565
lr:  [7.722771492524318e-05]
0.00020602556471364516
272.0370432745174 0.05604658546366277 0.05812659234452683

840 :  0.0502724248295029
lr:  [7.345206201812147e-05]
-5.602043274105772e-05
-1011.5491815401085 0.05666742288873963 0.055372133816592395
```

```
850 :  0.06250190953724086
lr:  [6.986100028903547e-05]
-0.0054229916431339205
-11.068894183472198 0.06002652065570339 0.05445885293325409

860 :  0.02783414932588736
lr:  [6.644550509937384e-05]
-0.00047894086416329015
-96.29284499600003 0.046118578395126 0.04524165657589523

870 :  0.006940356044409176
lr:  [6.319699302392957e-05]
-0.00018939060684876303
-165.44709492638762 0.03133412570947346 0.03806879031433104

880 :  0.019587437839557728
lr:  [6.0107300280034106e-05]
-0.0005028604650173042
-61.37570804731522 0.030863417089439234 0.0362935888049736

890 :  0.025722599712510903
lr:  [5.716866221128857e-05]
-3.820132514853441e-06
-8000.781102090743 0.030564044032321793 0.034784406886009187

900 :  0.0322847507117937
lr:  [5.437369377433232e-05]
0.0005138538278905412
40.569211531143196 0.020846644639779015 0.029592168188537465

910 :  0.020767876498090723
lr:  [5.171537097961115e-05]
-0.0002769742130941784
-74.45432593377554 0.020621928336964957 0.027698653744029186

920 :  0.019134459869625666
lr:  [4.9187013239503754e-05]
-0.0004252730170264838
-27.489669269459633 0.011690614587283314 0.024424663222356077

930 :  0.009908039262518287
lr:  [4.678226657944606e-05]
-0.00028284344423030143
-34.4765793338509 0.00975147444406562 0.02266598093979216

940 :  0.015727105690166353
lr:  [4.4495087669861456e-05]
-5.5392191834038185e-05
```

```
-118.50458710581304 0.006564228822178684 0.019594865461462177

950 :  0.021689860328721503
lr:  [4.2319728638767885e-05]
0.00023100983642903295
27.549742010018583 0.00636426139539645 0.01843003956822213

960 :  0.017799837801915904
lr:  [4.0250722626894584e-05]
-5.618530297081689e-05
-101.28955721924635 0.005690984460143249 5 0.0173106734980441

970 :  0.011858415504684671
lr:  [3.8282870049007304e-05]
-0.00013107946019803437
-38.730161280479635 0.005076728634028082 0.01591177359262171

980 :  0.01399037465841199
lr:  [3.641122552691552e-05]
-0.00010162062577104974
-44.91435094501694 0.004564224449133161 0.014651490217268779

990 :  0.01243300869440039
lr:  [3.463108546132327e-05]
-9.320005077589923e-05
-42.88030893873289 0.003996446970376151 0.013643077070941218

1000 :  0.012766406335867942
lr:  [3.293797621129047e-05]
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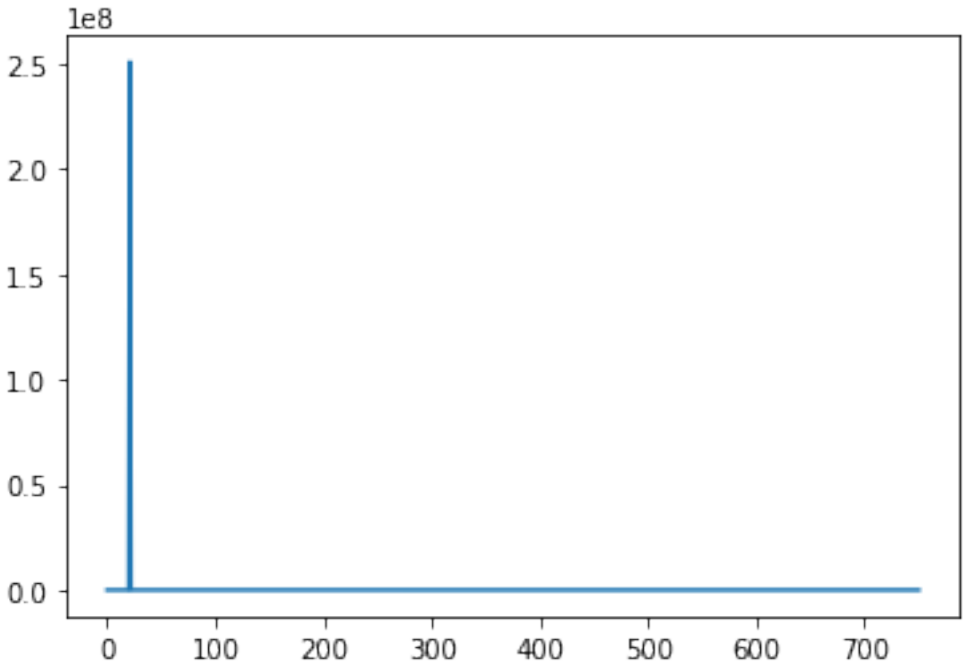
1e8
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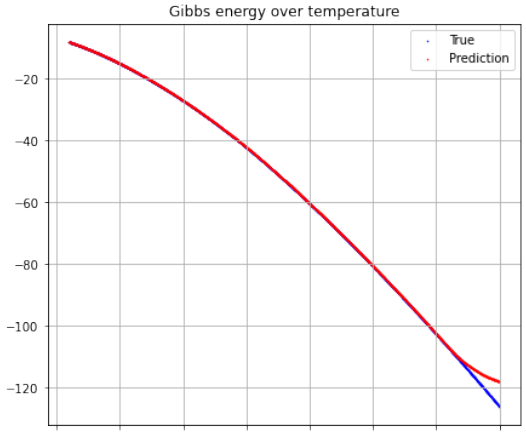
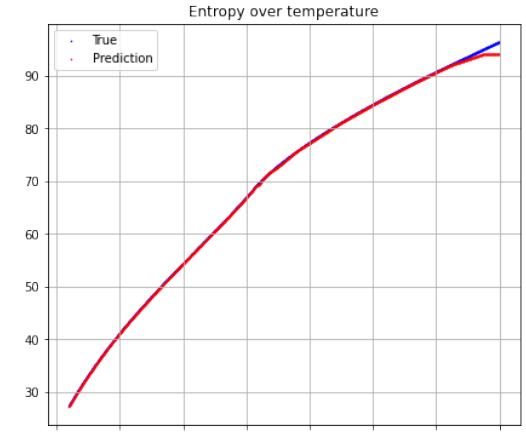
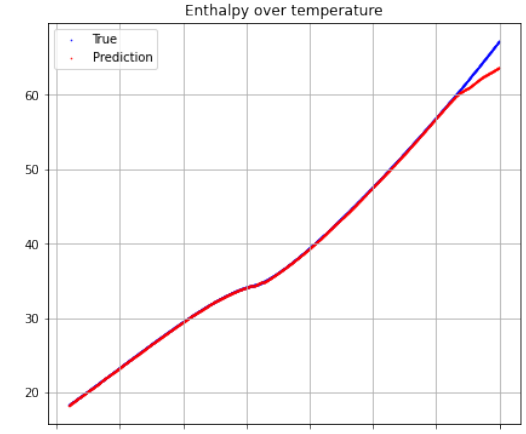
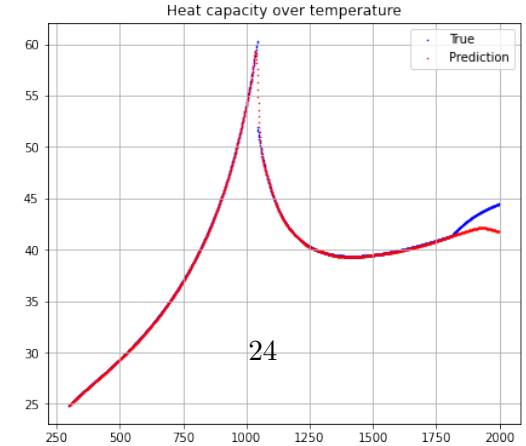
2.0
1.5
1.0
0.5
0.0
0
100
200
300
400
500
600
700


Gibbs energy over temperature
True
Prediction
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
90
80
70
60
50
40
30


Enthalpy over temperature
True
Prediction
60
50
40
30
20


Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

```
1010 :  0.007974019879475236
lr:  [3.132764285159898e-05]
-4.6918653094266696e-05
-76.4310815583854 0.0035860434012574896 0.011583200195396784

1020 :  0.008734084013849498
lr:  [2.9796038479769403e-05]
-0.00018099542421314132
-19.80004469206324 0.0035837174884791427 0.010838637704165495

1030 :  0.004990351037122309
lr:  [2.8339314045856632e-05]
-4.905128335187431e-05
-68.05470000138492 0.0033381703731947326 0.010077590173944677

1040 :  0.00960212085628882
lr:  [2.695380867946518e-05]
3.449457901891099e-05
90.53282794502555 0.003122891787355157 0.009627880152955185

1050 :  0.004423963790759444
lr:  [2.563604048967558e-05]
-4.806708418574105e-05
-62.97190251169978 0.0030268757393661517 0.009055706627026667

1060 :  0.008454092409616957
lr:  [2.438269781476115e-05]
-3.0089580362067228e-05
-83.61301819162477 0.002515880630191883 0.008558423425303772

1070 :  0.005269415139143045
lr:  [2.319063089970496e-05]
-0.00011175097985744324
-20.351493853896653 0.0023914999434601946 0.008061911377299112

1080 :  0.010546544933458791
lr:  [2.2056843980601938e-05]
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-38.294814707099114 0.0022546371589188454 0.007720743777967679

1090 :  0.005653469959118714
lr:  [2.0978487756053488e-05]
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```

```
1100 :  0.0073512559135754905
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lr:  [1.8977359884438732e-05]
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1120 :  0.005807642960765709
lr:  [1.8049559235584425e-05]
-4.578892943024836e-05
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lr:  [1.7167118639406374e-05]
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1140 :  0.005679117216883848
lr:  [1.6327820448847178e-05]
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lr:  [1.5529555437324735e-05]
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1160 :  0.004337814167956822
lr:  [1.4770317498069367e-05]
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lr:  [1.404819860260963e-05]
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1180 :  0.0037776520640666906
lr:  [1.336138400573712e-05]
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1190 :  0.0038279602934683985
lr:  [1.2708147684899912e-05]
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```
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1200 :  0.004483794395734246
lr:  [1.2086848002563453e-05]
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1210 :  0.0034261823806446047
lr:  [1.1495923580638079e-05]
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1220 :  0.004506817076859685
lr:  [1.0933889376605226e-05]
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lr:  [1.0399332951481313e-05]
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1240 :  0.004705539644540598
lr:  [9.890910920240393e-06]
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lr:  [9.40734557577517e-06]
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```

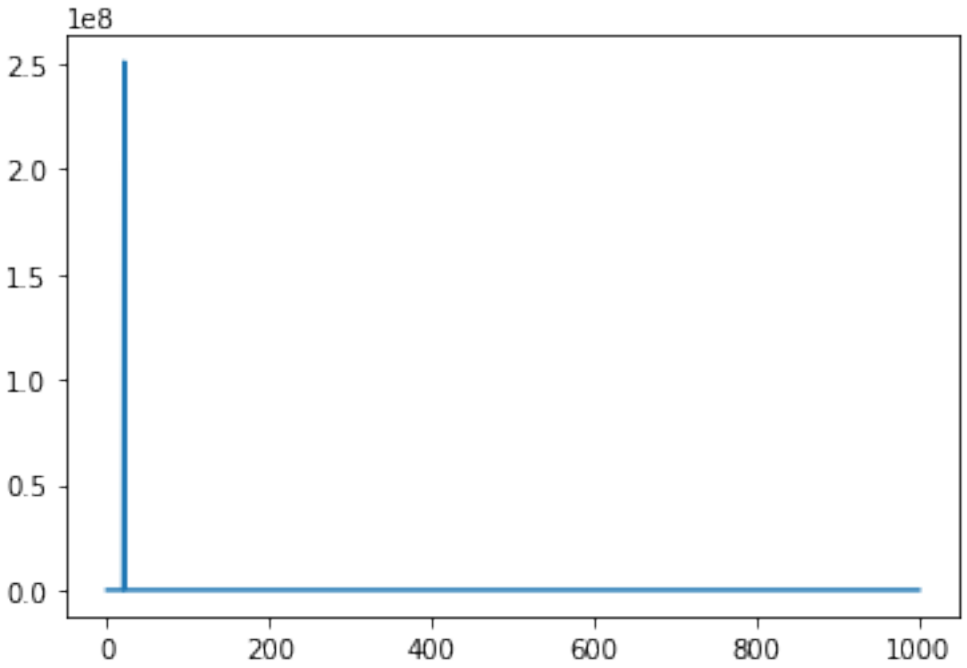
1e8
2.5
2.0
1.5
1.0
0.5
0.0
0
200
400
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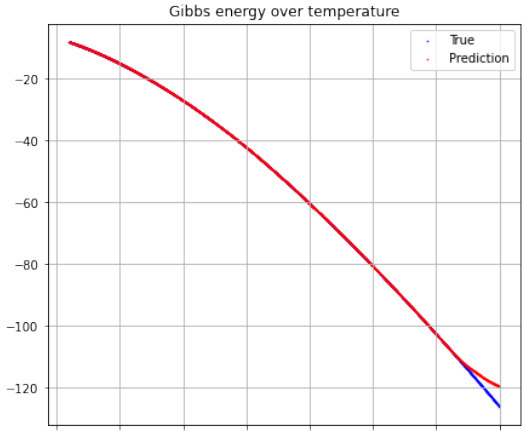
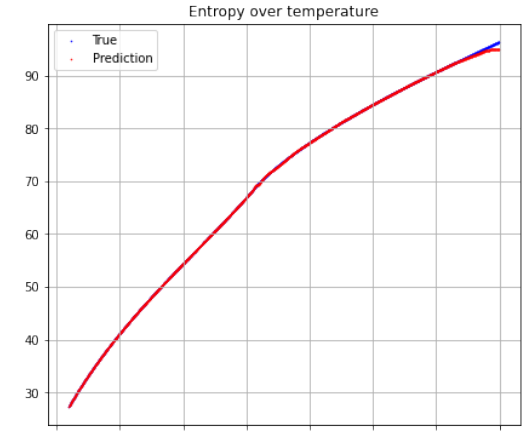
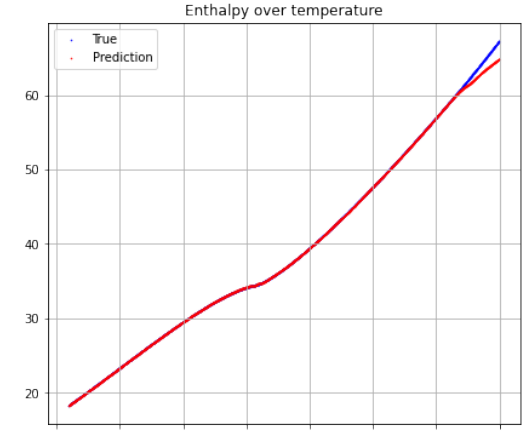
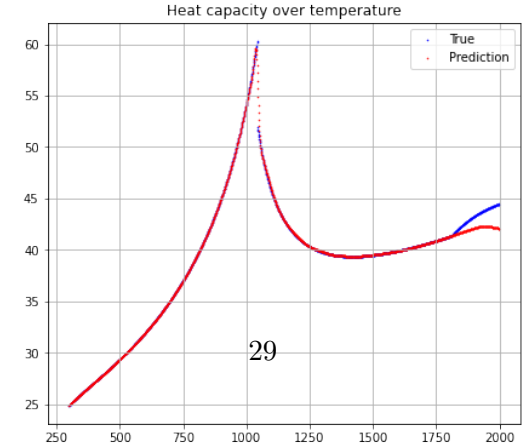
800
1000


Gibbs energy over temperature
True
Prediction
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
90
80
70
60
50
40
30


Enthalpy over temperature
True
Prediction
60
50
40
30
20


Heat capacity over temperature
True
Prediction
60
55
50
45
40
35
30
25
250
500
750
1000
1250
1500
1750
2000

```
1260 :  0.0037393475921514135
lr:  [8.947421677912122e-06]
-2.6260548885784998e-05
-16.434948667879297 0.00043159077292821127 0.003724183763590796

1270 :  0.0036851062730420383
lr:  [8.509983399411275e-06]
1.5311917253662235e-05
24.419784123136484 0.00037391371384576063 0.003609739612108872 5

1280 :  0.0035008402201735104
lr:  [8.09393142127561e-06]
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-44.78689694518175 0.00037950039659154087 0.003563462514760128

1290 :  0.0034324304344506385
lr:  [7.698220170070455e-06]
-2.0582423736277942e-05
-15.727781370128383 0.00032371586059152044 0.003452197071940949

1300 :  0.0032962273243659487
lr:  [7.3218551903099484e-06]
-1.1476548487592972e-05
-27.360294914616595 0.00031400175122244076 0.0033891266510278606
```
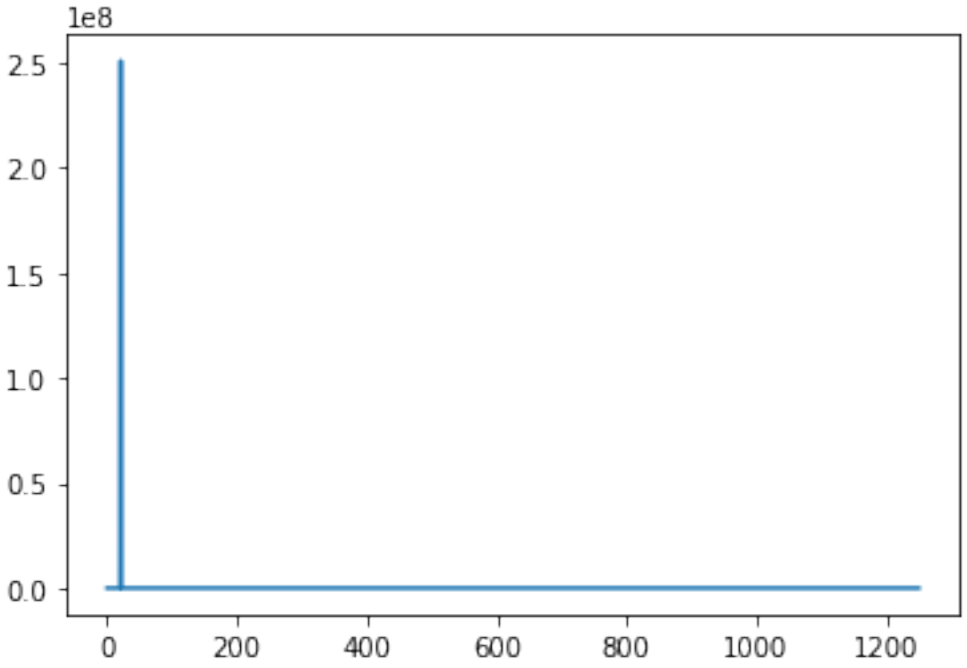

```
---------------------------------------------------------------------------
KeyboardInterrupt                         Traceback (most recent call last)
<ipython-input-239-dbdce5ac5a0c> in <module>
----> 1 losses, best_net = train(net, dataloader, optimizer=optimizer,␣
 ↪scheduler=scheduler, loss_func=loss_func, nr_epochs=nr_epochs)

<ipython-input-224-07be3a1041fc> in train(net, dataloader, optimizer, scheduler␣
 ↪loss_func, nr_epochs)
     33     for i in range(nr_epochs):
     34         #print('-----\nEpoch %i:\n' % i)
---> 35         loss = epoch(net, dataloader, loss_func, optimizer, scheduler)
     36         losses.append(loss)
     37

<ipython-input-224-07be3a1041fc> in epoch(net, dataloader, loss_func, optimizer␣
 ↪scheduler)
     14         # Backward pass
     15         net.zero_grad()
---> 16         loss.backward()
```

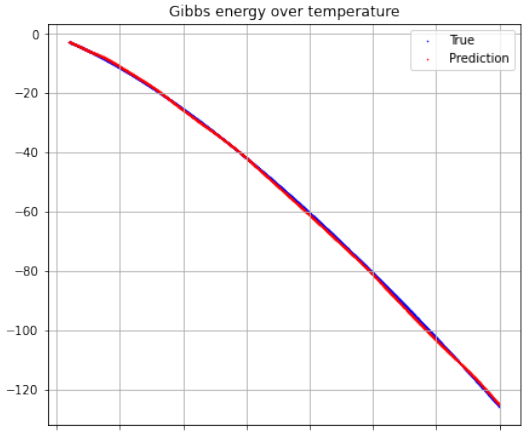
```
     17         optimizer.step()
     18         epoch_losses[i] = loss

~\anaconda3\envs\5_Programmcodes\lib\site-packages\torch\_tensor.py in␣
↪backward(self, gradient, retain_graph, create_graph, inputs)
    305                 create_graph=create_graph,
    306                 inputs=inputs)
--> 307         torch.autograd.backward(self, gradient, retain_graph,␣
↪create_graph, inputs=inputs)
    308
    309     def register_hook(self, hook):

~\anaconda3\envs\5_Programmcodes\lib\site-packages\torch\autograd\__init__.py i␣
↪backward(tensors, grad_tensors, retain_graph, create_graph, grad_variables,␣
↪inputs)
    152         retain_graph = create_graph
    153
--> 154     Variable._execution_engine.run_backward(
    155         tensors, grad_tensors_, retain_graph, create_graph, inputs,
    156         allow_unreachable=True, accumulate_grad=True)  #␣
↪allow_unreachable flag

KeyboardInterrupt:
```

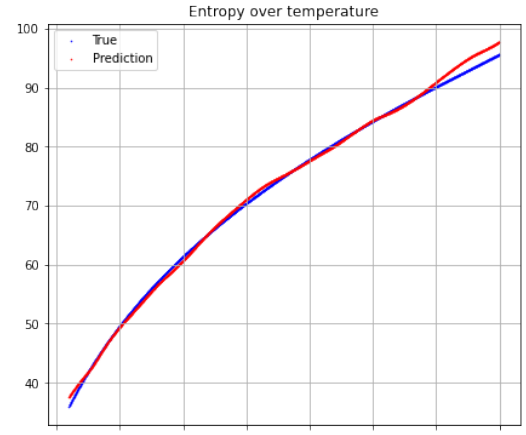


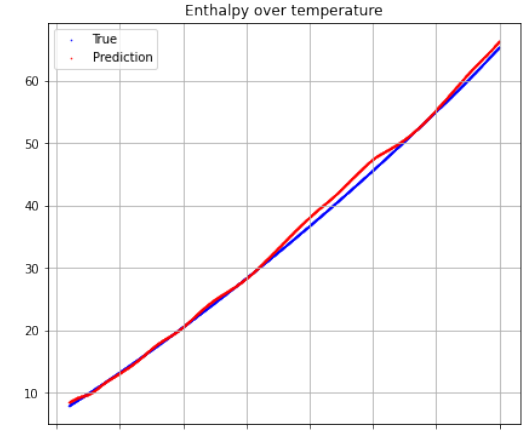
[ ]:
```
plt.plot(losses[1400:])
```

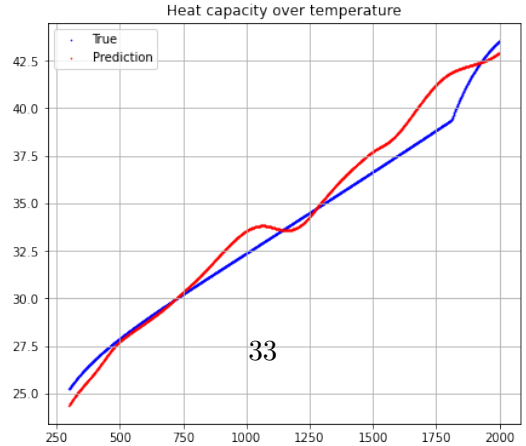
[240]:
```
#torch.save(net, 'Fe.pth')
```

[235]:
```
ph = PlotHandler()

ph.properties_temp_modified_new(net, ['Fe'], 'FCC_A1', start_temp=200,␣
↪end_temp=2000)
```


Gibbs energy over temperature
True
Prediction
0
−20
−40
−60
−80
−100
−120


Entropy over temperature
True
Prediction
100
90
80
70
60
50
40


Enthalpy over temperature
True
Prediction
60
50
40
30
20
10


Heat capacity over temperature
True
Prediction
42.5
40.0
37.5
35.0
32.5
30.0
27.5
25.0
250
500
750
1000
1250
1500
1750
2000

[ ]: