Final Project

This notebook is adapted from here:
https://aiqm.github.io/torchani/examples/nnp_training.html

Checkpoint 1: Data preparation

1. Create a working directory: `/global/scratch/users/[USER_NAME]/[DIR_NAME]`. Replace the [USER_NAME] with yours and specify a [DIR_NAME] you like.
2. Copy the Jupyter Notebook to the working directory
3. Download the ANI dataset `ani_dataset_gdb_s01_to_s04.h5` from bCourses and upload it to the working directory

In [1]:
```
import warnings
warnings.filterwarnings("ignore", category=UserWarning)
import numpy as np
from tqdm import tqdm
import torch
import torch.nn as nn
import torchani

print(torch.__version__)
print(torchani.__version__)
```

```
2.2.2
2.2.4
```

Use GPU

In [2]:
```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)
```

```
cuda
```

Set up AEV computer

AEV: Atomic Environment Vector (atomic features)

Ref: Chem. Sci., 2017, 8, 3192

In [3]:
```
def init_aev_computer():
    Rcr = 5.2
    Rca = 3.5
    EtaR = torch.tensor([16], dtype=torch.float, device=device)
    ShfR = torch.tensor([
        0.900000, 1.168750, 1.437500, 1.706250,
        1.975000, 2.243750, 2.512500, 2.781250,
        3.050000, 3.318750, 3.587500, 3.856250,
        4.125000, 4.393750, 4.662500, 4.931250
    ], dtype=torch.float, device=device)


    EtaA = torch.tensor([8], dtype=torch.float, device=device)
    Zeta = torch.tensor([32], dtype=torch.float, device=device)
    ShfA = torch.tensor([0.90, 1.55, 2.20, 2.85], dtype=torch.float, device=
    ShfZ = torch.tensor([
        0.19634954, 0.58904862, 0.9817477, 1.37444680,
        1.76714590, 2.15984490, 2.5525440, 2.94524300
    ], dtype=torch.float, device=device)

    num_species = 4
    aev_computer = torchani.AEVComputer(
        Rcr, Rca, EtaR, ShfR, EtaA, Zeta, ShfA, ShfZ, num_species
    )
    return aev_computer

aev_computer = init_aev_computer()
aev_dim = aev_computer.aev_length
print(aev_dim)
```

```
384
```

Prepare dataset & split

In [4]:
```
def load_ani_dataset(dspath):
    self_energies = torch.tensor([
        0.500607632585, -37.8302333826,
        -54.5680045287, -75.0362229210
    ], dtype=torch.float, device=device)
    energy_shifter = torchani.utils.EnergyShifter(None)
    species_order = ['H', 'C', 'N', 'O']

    dataset = torchani.data.load(dspath)
    dataset = dataset.subtract_self_energies(energy_shifter, species_order)
    dataset = dataset.species_to_indices(species_order)
    dataset = dataset.shuffle()
    return dataset

dataset = load_ani_dataset("ani_gdb_s01_to_s04.h5")
# Use dataset.split method to do split
train_data, val_data, test_data = dataset.split(.8, .1, .1)
```

Batching

```
In [5]: batch_size = 8192
        # use dataset.collate(...).cache() method to do batching
        train_data_loader = train_data.collate(batch_size).cache()
        val_data_loader = val_data.collate(batch_size).cache()
        test_data_loader = test_data.collate(batch_size).cache()
```

Torchani API

```
In [6]: class AtomicNet(nn.Module):
            def __init__(self):
                super().__init__()
                self.layers = nn.Sequential(
                    nn.Linear(384, 128),
                    nn.ReLU(),
                    nn.Linear(128, 1)
                )

            def forward(self, x):
                return self.layers(x)

        net_H = AtomicNet()
        net_C = AtomicNet()
        net_N = AtomicNet()
        net_O = AtomicNet()

        # ANI model requires a network for each atom type
        # use torch.ANIModel() to compile atomic networks
        ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
        model = nn.Sequential(
            aev_computer,
            ani_net
        ).to(device)
```

```
In [7]: # train_data_batch = next(iter(train_data_loader))

        for train_data_batch in train_data_loader:
            loss_func = nn.MSELoss()
            species = train_data_batch['species'].to(device)
            coords = train_data_batch['coordinates'].to(device)
            true_energies = train_data_batch['energies'].to(device).float()
            _, pred_energies = model((species, coords))
            loss = loss_func(true_energies, pred_energies)
            print(loss)
            break
```

```
tensor(0.0355, device='cuda:0', grad_fn=<MseLossBackward0>)
```

Checkpoint 2

In [8]:
```
coords.shape[0]
train_epoch_loss = 0.0

loss_func = nn.MSELoss()
batch_loss = loss_func(true_energies, pred_energies)
batch_importance = coords.shape[0] / len(train_data)
train_epoch_loss += batch_loss.detach().cpu().item() * batch_importance

print(train_epoch_loss)
```

```
0.0004199363558073355
```

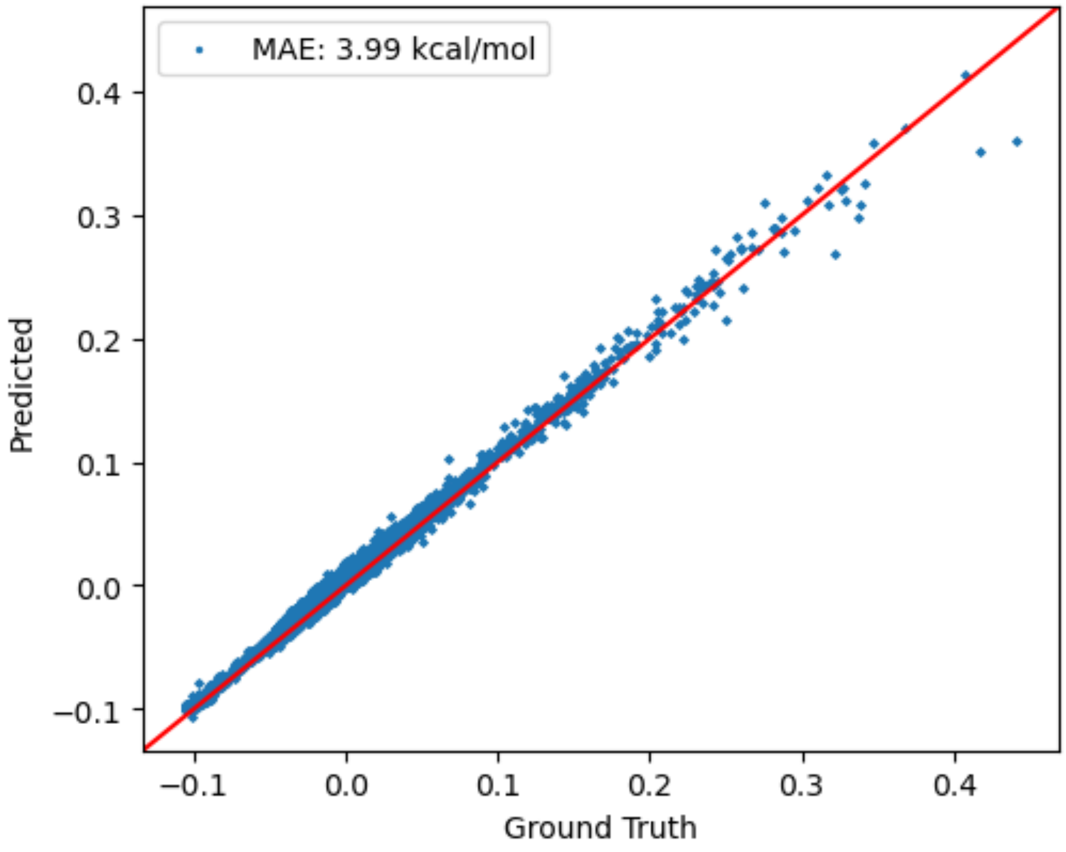
In [9]:
```
from torch.utils.data import DataLoader
import matplotlib.pyplot as plt
```

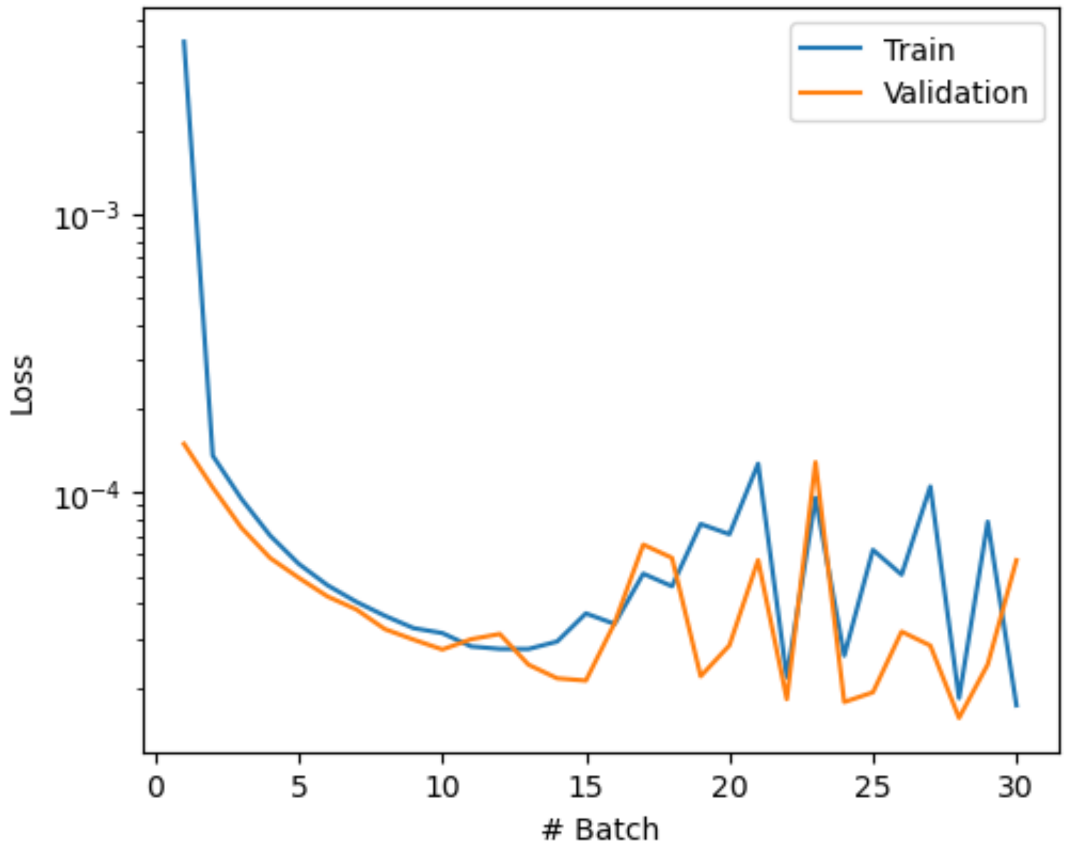
In [10]:
```
class ANITrainer:
    def __init__(self, model, batch_size, learning_rate, epoch, l2):
        self.model = model

        num_params = sum(item.numel() for item in model.parameters())
        print(f"{model.__class__.__name__} - Number of parameters: {num_para

        self.batch_size = batch_size
        self.optimizer = torch.optim.Adam(model.parameters(), learning_rate,
        self.epoch = epoch

    def train(self, train_data, val_data, early_stop=True, draw_curve=True):
        self.model.train()

        # init data loader
        print("Initialize training data...")
        train_data_loader = train_data.collate(batch_size).cache()

        # definition of loss function: MSE is a good choice!
        loss_func = nn.MSELoss()

        # record epoch losses
        train_loss_list = []
        val_loss_list = []
        lowest_val_loss = np.inf

        for i in tqdm(range(self.epoch), leave=True):
            train_epoch_loss = 0.0
            for train_data_batch in train_data_loader:

                # compute energies
                species = train_data_batch['species'].to(device)
                coords = train_data_batch['coordinates'].to(device)
                true_energies = train_data_batch['energies'].to(device).floa
                _, pred_energies = model((species, coords))

                # compute loss
                batch_loss = loss_func(true_energies, pred_energies)

                # do a step
                self.optimizer.zero_grad()
                batch_loss.backward()
                self.optimizer.step()

                batch_importance = coords.shape[0] / len(train_data)
                train_epoch_loss += batch_loss.detach().cpu().item() * batch

            # use the self.evaluate to get loss on the validation set
            if (i == (self.epoch - 1)):
                val_epoch_loss = self.evaluate(val_data, draw_plot = True)
            else:
                val_epoch_loss = self.evaluate(val_data)

            # append the losses
            train_loss_list.append(train_epoch_loss)
            val_loss_list.append(val_epoch_loss)

            if early_stop:
                if val_epoch_loss < lowest_val_loss:
                    lowest_val_loss = val_epoch_loss
                    weights = self.model.state_dict()

        if draw_curve:
            fig, ax = plt.subplots(1, 1, figsize=(5, 4), constrained_layout=
            ax.set_yscale("log")
            # Plot train loss and validation loss
            ax.plot(range(1, len(train_loss_list) + 1), train_loss_list, lab
            ax.plot(range(1, len(val_loss_list) + 1), val_loss_list, label='
            ax.legend()
            ax.set_xlabel("# Batch")
            ax.set_ylabel("Loss")

        if early_stop:
            self.model.load_state_dict(weights)

        return train_loss_list, val_loss_list


    def evaluate(self, data, draw_plot=False):

        # init data loader
        data_loader = data.collate(batch_size).cache()

        # init loss function
        loss_func = nn.MSELoss()
        total_loss = 0.0
        if draw_plot:
            true_energies_all = []
            pred_energies_all = []

        with torch.no_grad():
            for batch_data in data_loader:

                # compute energies
                species = train_data_batch['species'].to(device)
                coords = train_data_batch['coordinates'].to(device)
                true_energies = train_data_batch['energies'].to(device).floa
                _, pred_energies = model((species, coords))


                # compute loss
                batch_loss = loss_func(true_energies, pred_energies)

                batch_importance = coords.shape[0] / len(data)
                total_loss += batch_loss.detach().cpu().item() * batch_impor

                if draw_plot:
                    true_energies_all.append(true_energies.detach().cpu().nu
                    pred_energies_all.append(pred_energies.detach().cpu().nu

        if draw_plot:
            true_energies_all = np.concatenate(true_energies_all)
            pred_energies_all = np.concatenate(pred_energies_all)
            # Report the mean absolute error
            # The unit of energies in the dataset is hartree
            # please convert it to kcal/mol when reporting the mean absolute
            # 1 hartree = 627.5094738898777 kcal/mol
            # MAE = mean(|true - pred|)
            hartree2kcalmol = 627.5094738898777 # changed
            mae = np.mean(np.abs(true_energies_all * hartree2kcalmol - pred_
            fig, ax = plt.subplots(1, 1, figsize=(5, 4), constrained_layout=
            ax.scatter(true_energies_all, pred_energies_all, label=f"MAE: {m
            ax.set_xlabel("Ground Truth")
            ax.set_ylabel("Predicted")
            xmin, xmax = ax.get_xlim()
            ymin, ymax = ax.get_ylim()
            vmin, vmax = min(xmin, ymin), max(xmax, ymax)
            ax.set_xlim(vmin, vmax)
            ax.set_ylim(vmin, vmax)
            ax.plot([vmin, vmax], [vmin, vmax], color='red')
            ax.legend()
            #print(mae)

        return total_loss
```

In [13]:
```
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

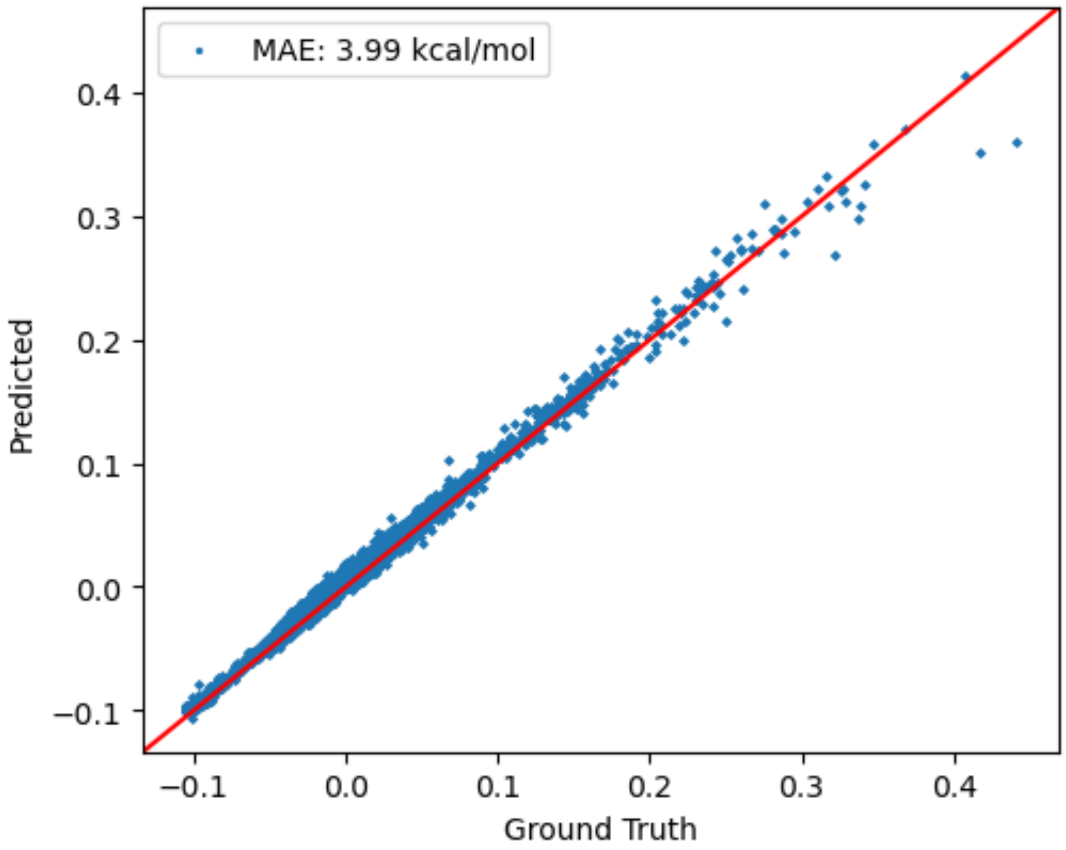
In [14]:
```
model = model

trainer = ANITrainer(model, learning_rate=1e-3, batch_size = 8192, epoch = 3

train_losses, val_losses = trainer.train(train_data, val_data)
```

```
Sequential - Number of parameters: 197636
Initialize training data...
100%|██████████| 30/30 [04:47<00:00,  9.57s/it]
```





```
In [15]: trainer.evaluate(test_data, draw_plot = True)

Out[15]: 5.7331837363884256e-05
```



In [16]:
```
print(train_losses)
```

```
[0.004150044536737322, 0.00013599351319533524, 9.514818989270177e-05, 7.0278
52081559144e-05, 5.559908003337367e-05, 4.661247391919525e-05, 4.06657865127
73615e-05, 3.621267203060398e-05, 3.270527230855875e-05, 3.1402471820477994e
-05, 2.812861814916419e-05, 2.755122388931103e-05, 2.7531479899193634e-05,
2.9291981469117514e-05, 3.693555873841545e-05, 3.3873674977873154e-05, 5.129
2386025111436e-05, 4.623098497962414e-05, 7.731075727434039e-05, 7.103601808
456633e-05, 0.00012720442190070373, 2.1829907562654332e-05, 9.59621303833095
9e-05, 2.6061130264811148e-05, 6.244133583872179e-05, 5.088604436045897e-05,
0.00010542876427378199, 1.8358793291461095e-05, 7.876913400413208e-05, 1.729
4839518349943e-05]
```

Checkpoint 3

The lowest loss after checkpoint 2 was 1.7294839518349943e-05, and the MAE was 3.99 kcal/mol for both validation and test data. Now I will optimize the loss and MAE by implementing regularization techniques and performing hyperparameter tuning. My approaches include: modifying the architecture in each atomic net, using more hidden layers, varying the hidden layer size, adding dropouts, changing activation function

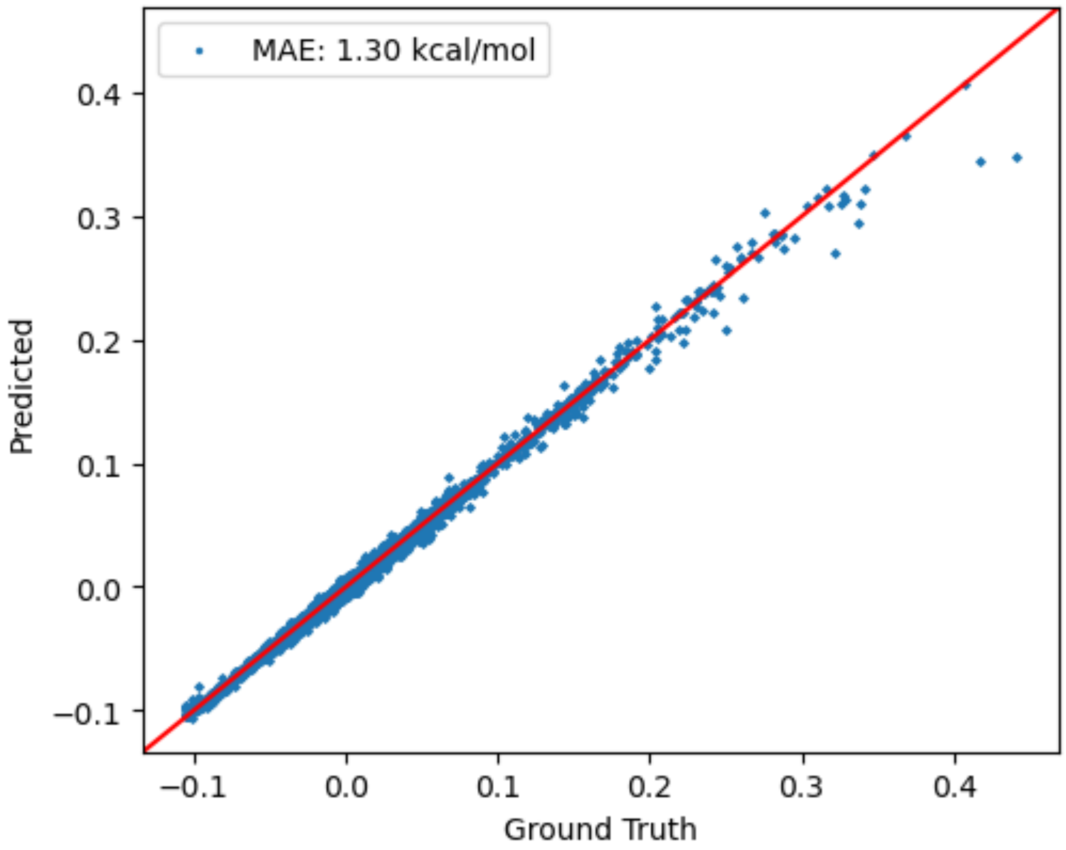
Iteration 1

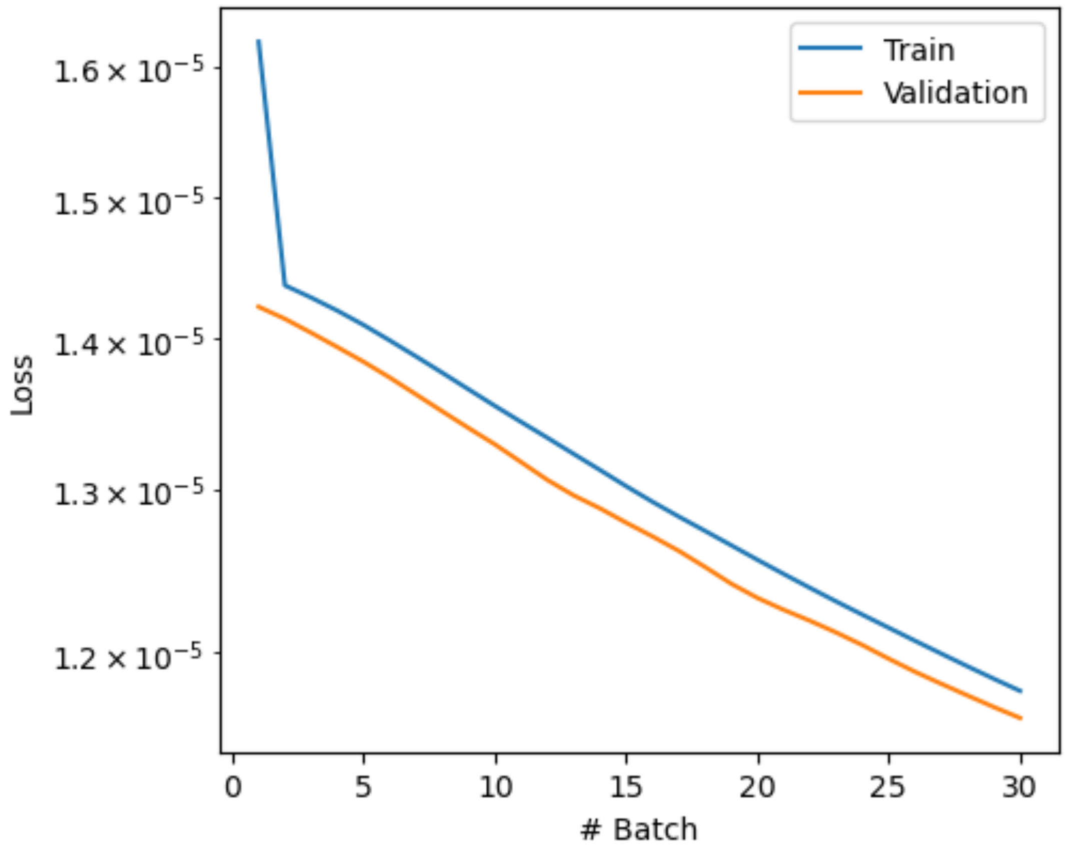
Here I decreased the learning rate from 1e-3 to 1e-5

```
In [17]: ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
         model = nn.Sequential(
             aev_computer,
             ani_net
         ).to(device)
```

```
In [18]: model = model

         # tried decreasing the learning rate
         trainer = ANITrainer(model, learning_rate=1e-5, batch_size = 8192, epoch = 3

         train_losses, val_losses = trainer.train(train_data, val_data)
```

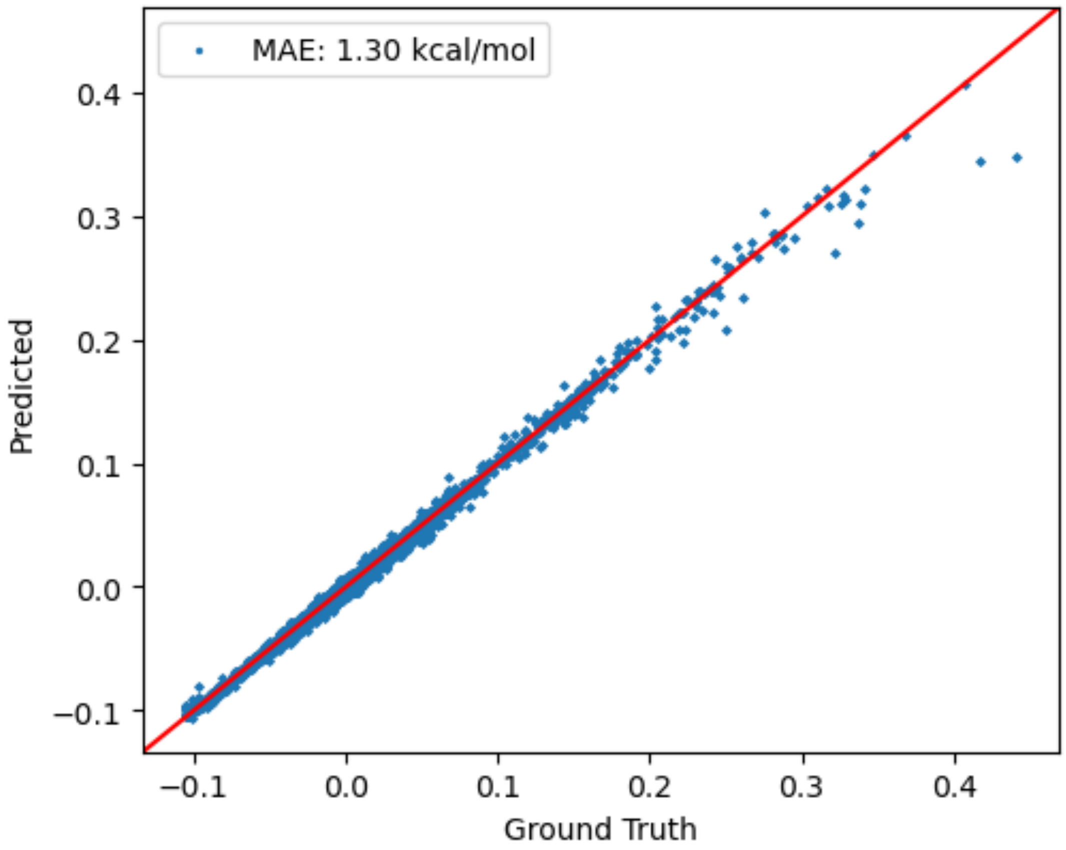
```
Sequential - Number of parameters: 197636
Initialize training data...
100%|██████████| 30/30 [04:55<00:00,  9.85s/it]
```





```
In [19]: trainer.evaluate(test_data, draw_plot = True)
```

```
Out[19]: 1.1618574713498447e-05
```



In [20]:
```
print(train_losses)
```

```
[1.6198787425184687e-05, 1.437100855824389e-05, 1.4284719865594101e-05, 1.41
93105494001543e-05, 1.409366437732297e-05, 1.3986305857150458e-05, 1.3877033
926014824e-05, 1.3766084715054987e-05, 1.3654304865283119e-05, 1.35442844073
60258e-05, 1.3437554973404667e-05, 1.3333548492603435e-05, 1.322821489480700
8e-05, 1.3124391283397342e-05, 1.3020091951700905e-05, 1.2920777155121306e-0
5, 1.2827279716368306e-05, 1.2737543308203968e-05, 1.2647523866215924e-05,
1.2557485454078932e-05, 1.2470214182097147e-05, 1.2385469280158987e-05, 1.23
02969178580005e-05, 1.2223159963160752e-05, 1.2145029925637953e-05, 1.206752
8187063236e-05, 1.1991593831423151e-05, 1.1917112312281973e-05, 1.1844411974
322837e-05, 1.1774181918935158e-05]
```

This gives a very optimal loss of 1.1774181918935158e-05, which is even less than what we had achieved in checkpoint 2. Furthermore, we have a validation and test MAE of 1.30 kcal/mol which is signinifcantly less than the MAE from iteration 1 of 3.99. Since the MAE for this iteration is less tha 2 kcal/mol, we can see that this model architecture is efficiently and accuratly predicts molecular preoperties.

Altering Hidden Layers and Number of Neurons

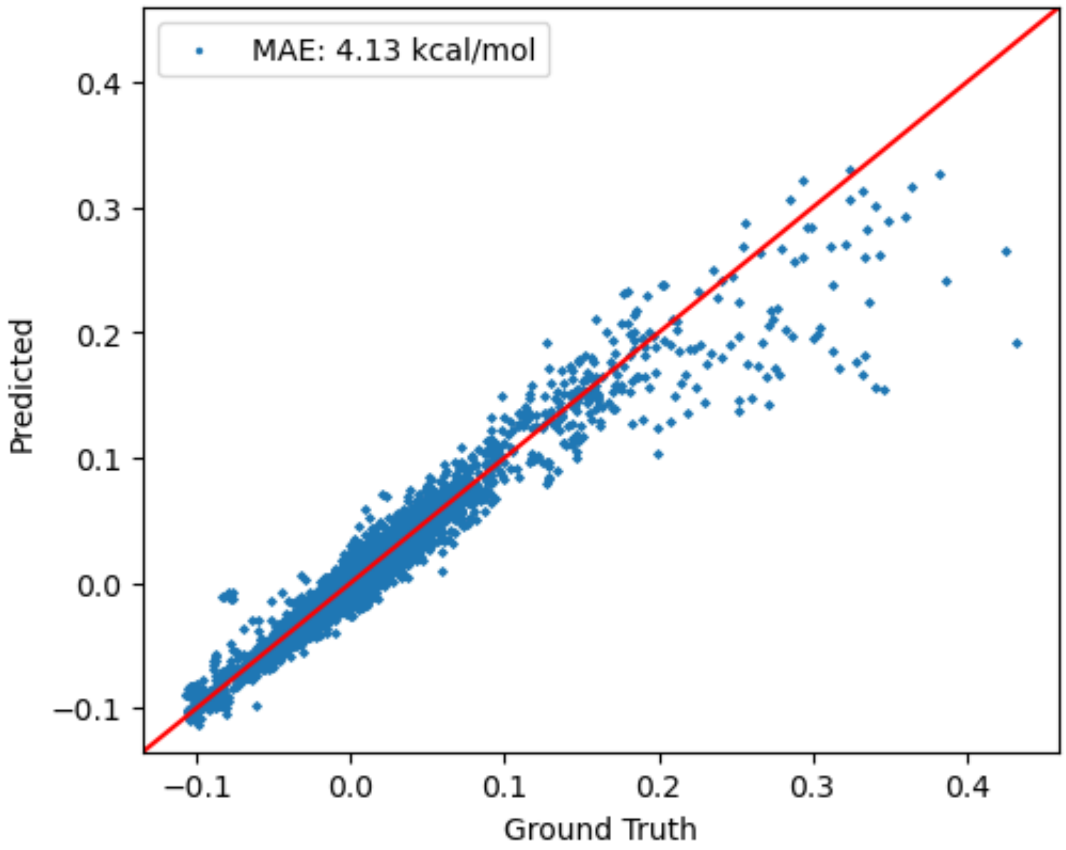
Iteration 2

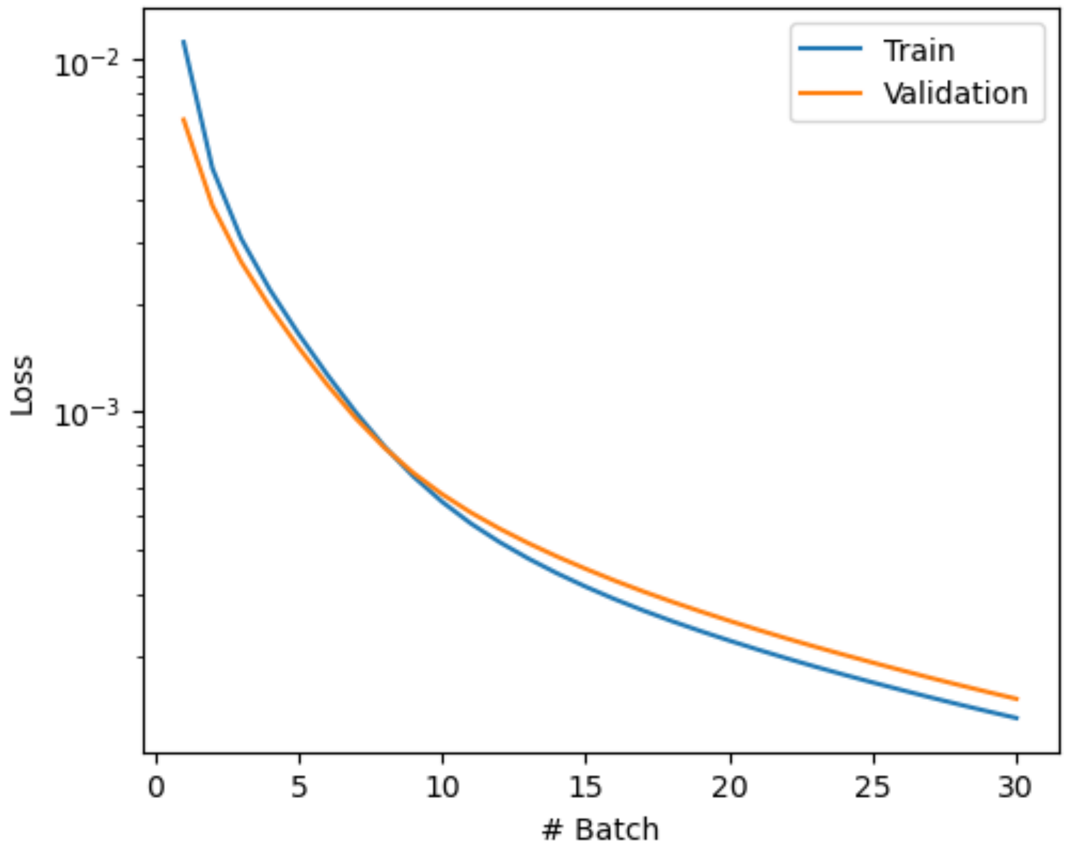
Here I change the hidden layer size to be 200 neurons.

In [27]:
```
# change hidden layer to 200 neurons
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 200),
            nn.ReLU(),
            nn.Linear(200, 1)
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torch.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [28]:
```
model = model

trainer = ANITrainer(model, learning_rate=1e-5, batch_size = 8192, epoch = 3

train_losses, val_losses = trainer.train(train_data, val_data)
```

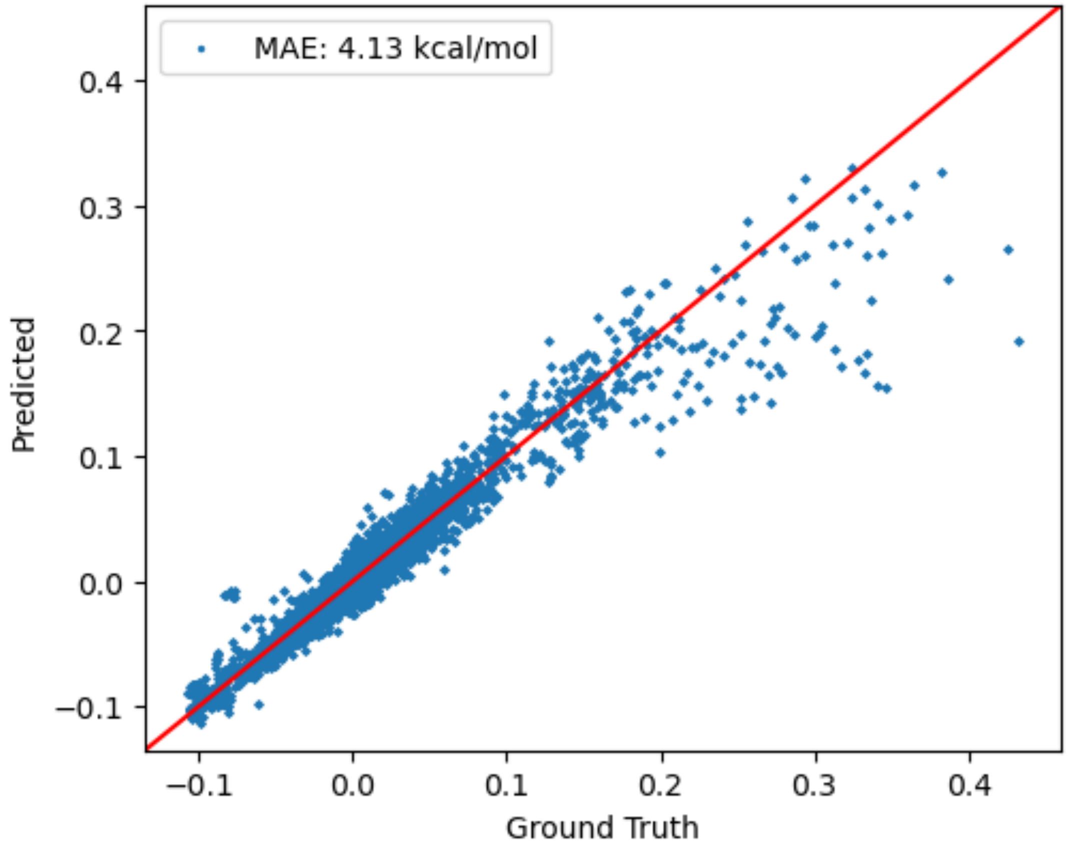
```
Sequential - Number of parameters: 308804
Initialize training data...
100%|██████████| 30/30 [05:15<00:00, 10.50s/it]
```


MAE: 4.13 kcal/mol
Predicted
Ground Truth
0.4
0.3
0.2
0.1
0.0
−0.1
−0.1
0.0
0.1
0.2
0.3
0.4


Train
Validation
Loss
10^{-2}
10^{-3}
# Batch
0
5
10
15
20
25
30

```
In [29]: trainer.evaluate(test_data, draw_plot = True)
```

```
Out[29]: 0.0001510852903961897
```



```
In [30]: print(train_losses)
```

```
[0.011198594086009303, 0.004904332405735425, 0.0030942654196581304, 0.002212
1939635551344, 0.001655802852550606, 0.0012665693233772789, 0.00098804594648
36882, 0.0007894237959531604, 0.0006494236399167477, 0.0005498852287692776,
0.0004771340878089664, 0.0004222732428181937, 0.0003792264057511114, 0.00034
41798974062128, 0.0003151930724736412 5, 0.00029070105561644 93, 0.00026971169
850084837, 0.0002515513059471340 3, 0.0002355815441843788, 0.0002213984195992
1885, 0.000208615520156008, 0.00019700053473018506, 0.00018650730068935957,
0.00017693778144532412, 0.0001681686502599739, 0.00016008687285793452, 0.000
1525658371898371, 0.0001456089711597646, 0.0001391919152983602, 0.0001332223
0234034257]
```

We can see that the lowest loss here is 0.00013322230234034257, which is not as optimale as Iteration 1. Both the validation and test MAE are 4.13.

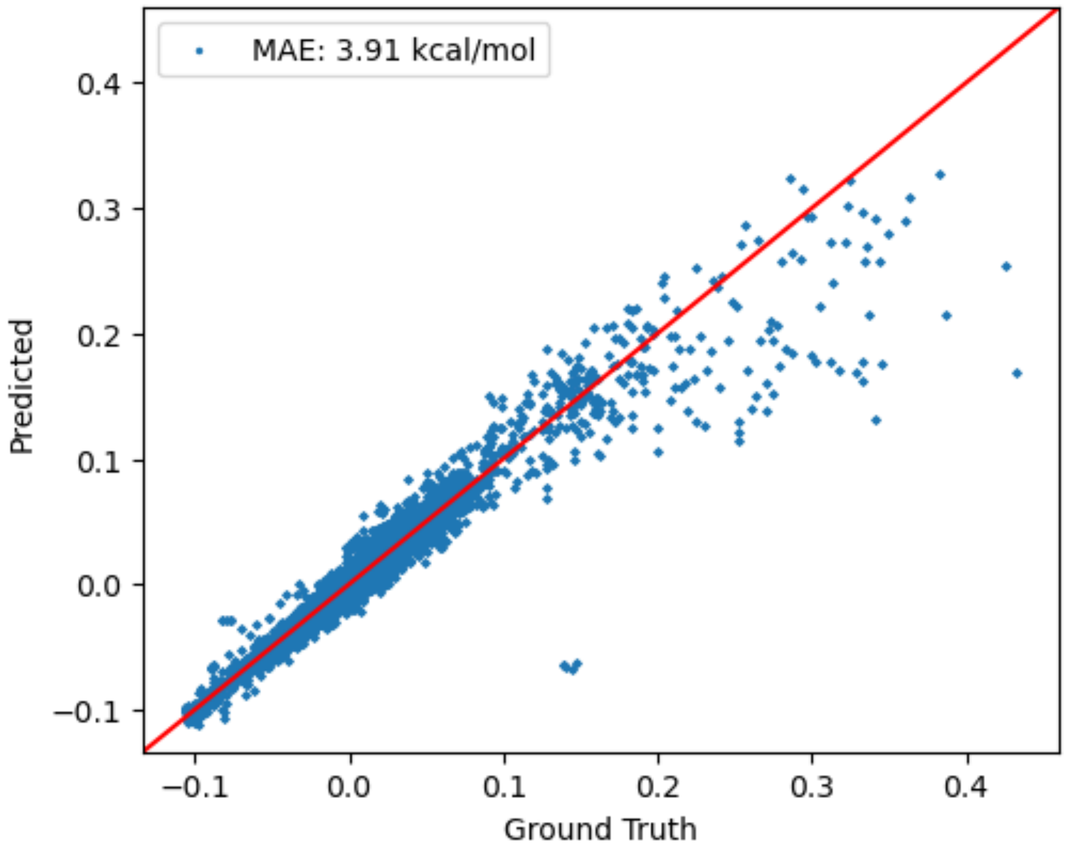
Iteration 3

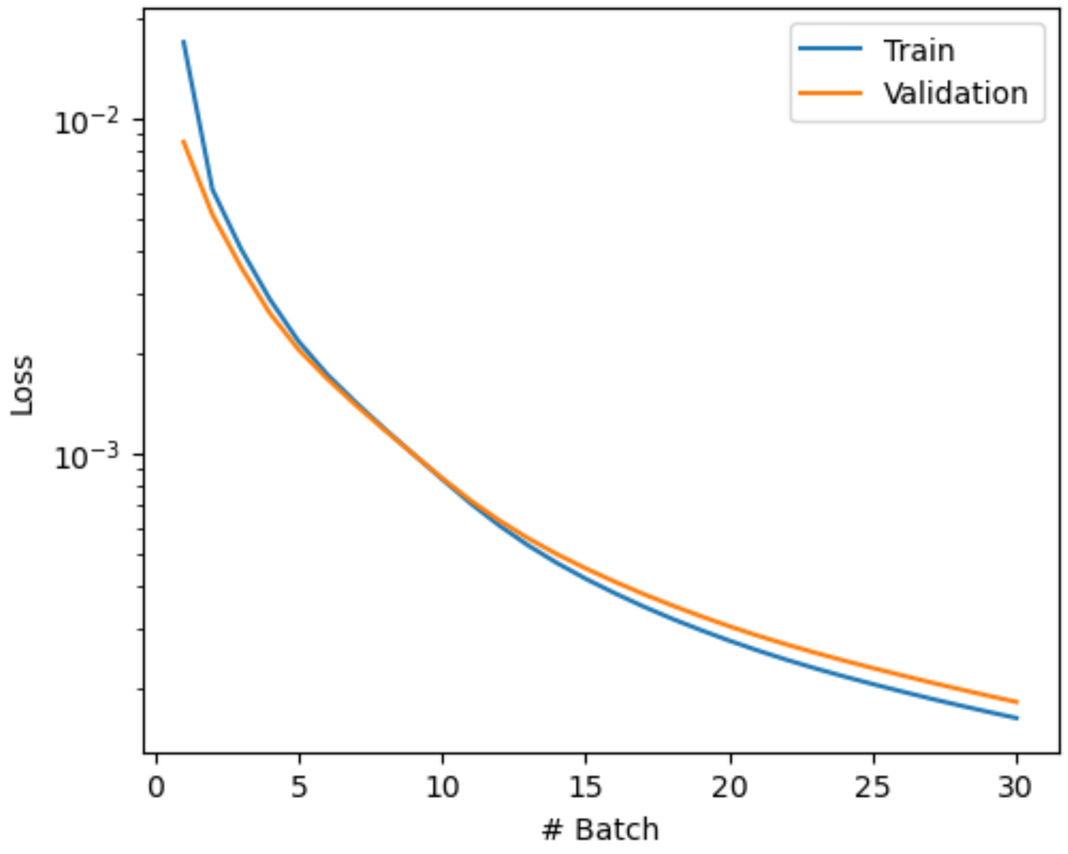
Here I add another hidden layer for total of 2 hidden layers

In [31]:
```
# change to 2 hidden layers
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 128),
            nn.ReLU(),
            nn.Linear(128, 64),
            nn.ReLU(),
            nn.Linear(64, 1)
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torch.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [32]:
```
model = model

trainer = ANITrainer(model, learning_rate=1e-5, batch_size = 8192, epoch = 3

train_losses, val_losses = trainer.train(train_data, val_data)
```

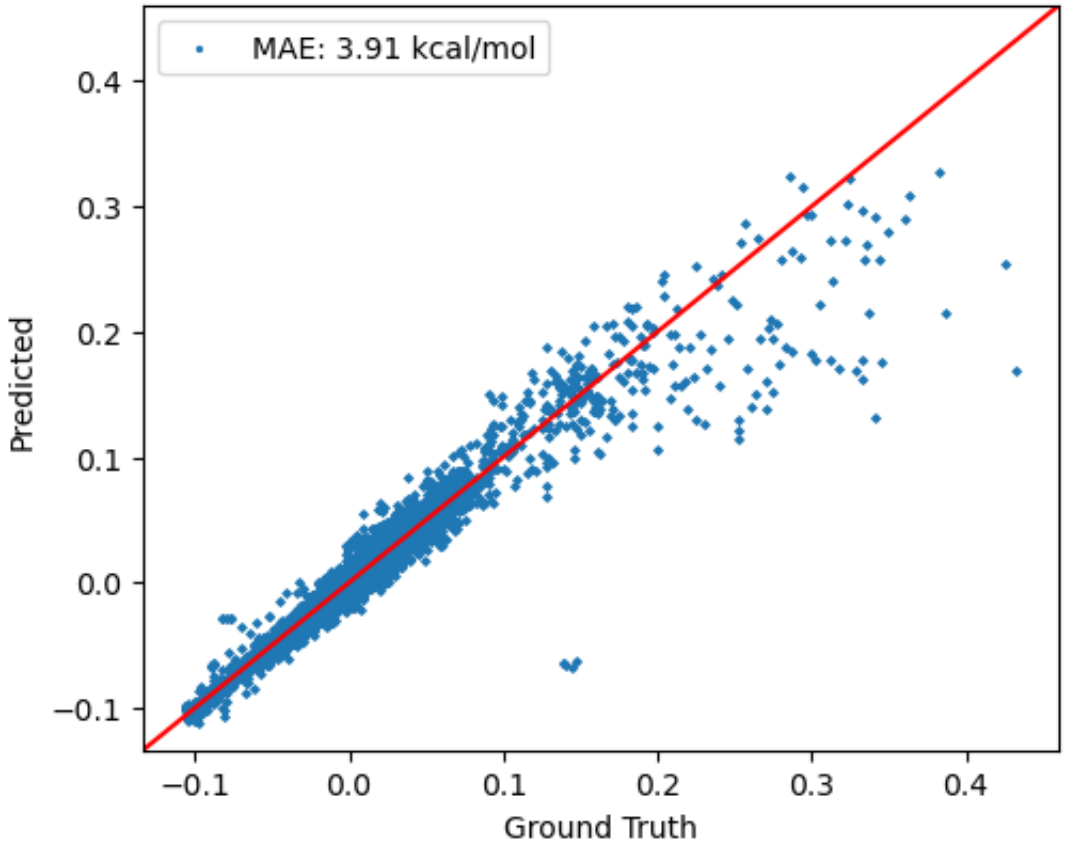
```
Sequential - Number of parameters: 230404
Initialize training data...
100%|██████████| 30/30 [04:56<00:00,  9.88s/it]
```


MAE: 3.91 kcal/mol
Predicted
Ground Truth
0.4
0.3
0.2
0.1
0.0
−0.1
−0.1
0.0
0.1
0.2
0.3
0.4


Train
Validation
Loss
10^{-2}
10^{-3}
# Batch
0
5
10
15
20
25
30

In [33]:
```
trainer.evaluate(test_data, draw_plot = True)
```

Out[33]:
```
0.00018131680013287472
```



In [34]:
```
print(train_losses)
```

```
[0.016902633900835327, 0.006151463566138277, 0.004080630323489097, 0.0028912
382810755764, 0.002164501003997744, 0.0017229005873061597, 0.001419564669807
1768, 0.0011846522954481072, 0.0009959653117935375, 0.0008389344439036669,
0.0007092813084363018, 0.0006091732172968584, 0.0005317302496779389, 0.00047
127280169100423, 0.0004229998762752826, 0.0003833631131530 6966, 0.0003498510
0296456504, 0.0003215336028427507, 0.0002974240786006 6213, 0.000276422869111
1021, 0.0002581598130783 2217, 0.0002422618553060 7145, 0.000228387511516819 5
8, 0.0002160682457105 9532, 0.0002050039899556 1942, 0.0001949501493045 7887,
0.0001857012934934 0076, 0.0001772792152086 0123, 0.0001695467715186 2892, 0.00
016239312862845572]
```

Similar to iterration 2, iteration 3 leads to a loss of 0.00016239312862845572. This is again not as optimal as iteration 1. The validation and test MAE are 3.91, which is slightly better than the MAE found in iteration 2.

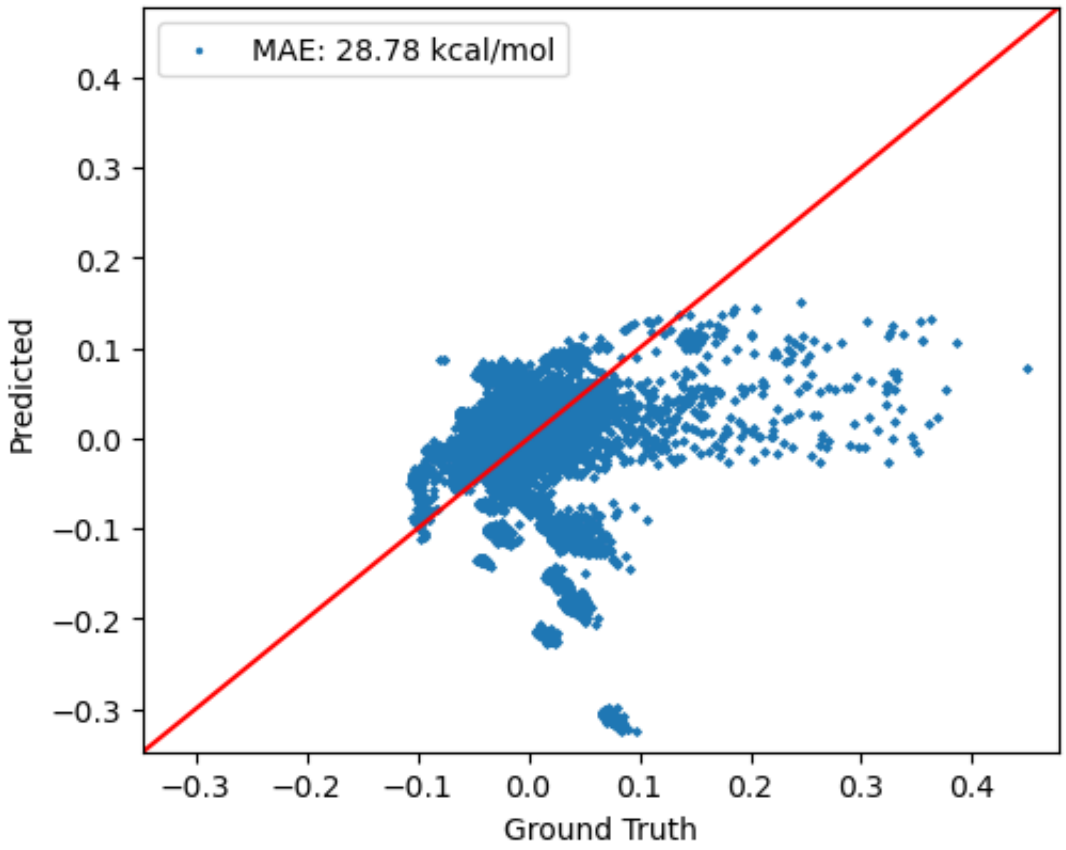
Iteration 4

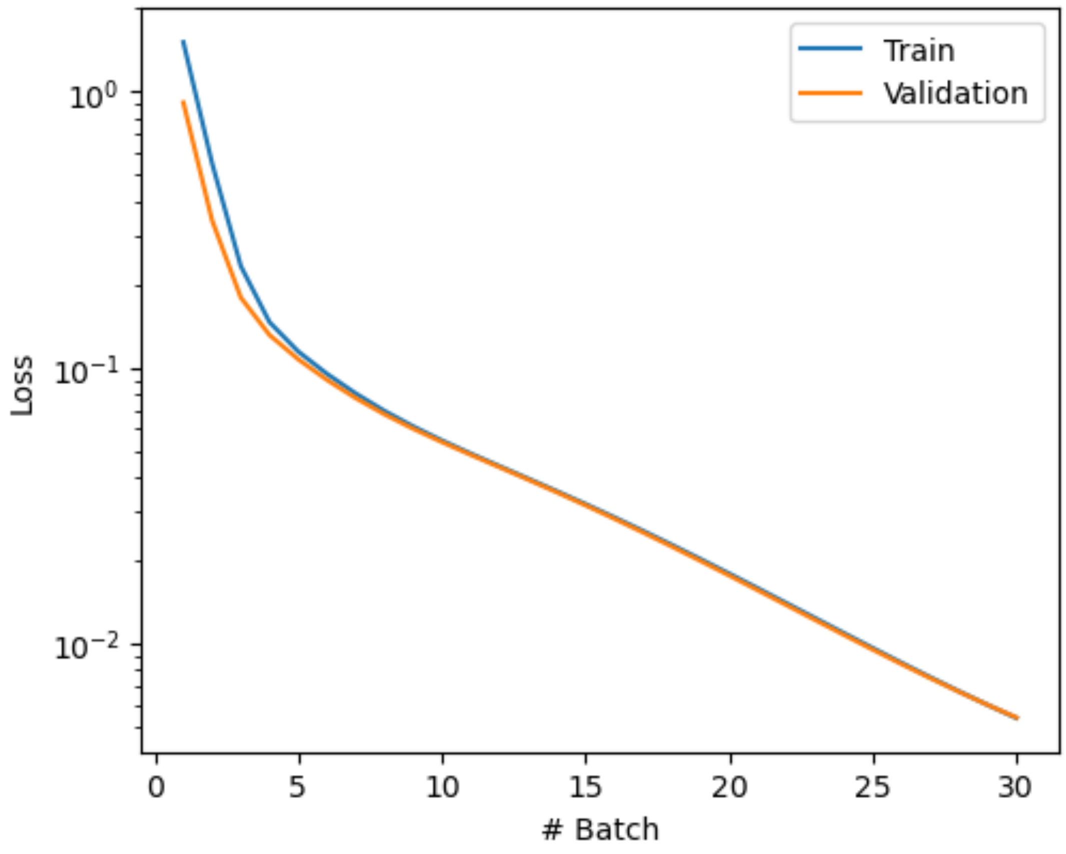
Now I will change activation function from ReLU to Sigmoid.

In [16]:
```
# change activation function
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 128),
            nn.Sigmoid(),
            nn.Linear(128, 1)
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torch.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [17]:
```
model = model

trainer = ANITrainer(model, learning_rate=1e-5, batch_size = 8192, epoch = 3

train_losses, val_losses = trainer.train(train_data, val_data)
```

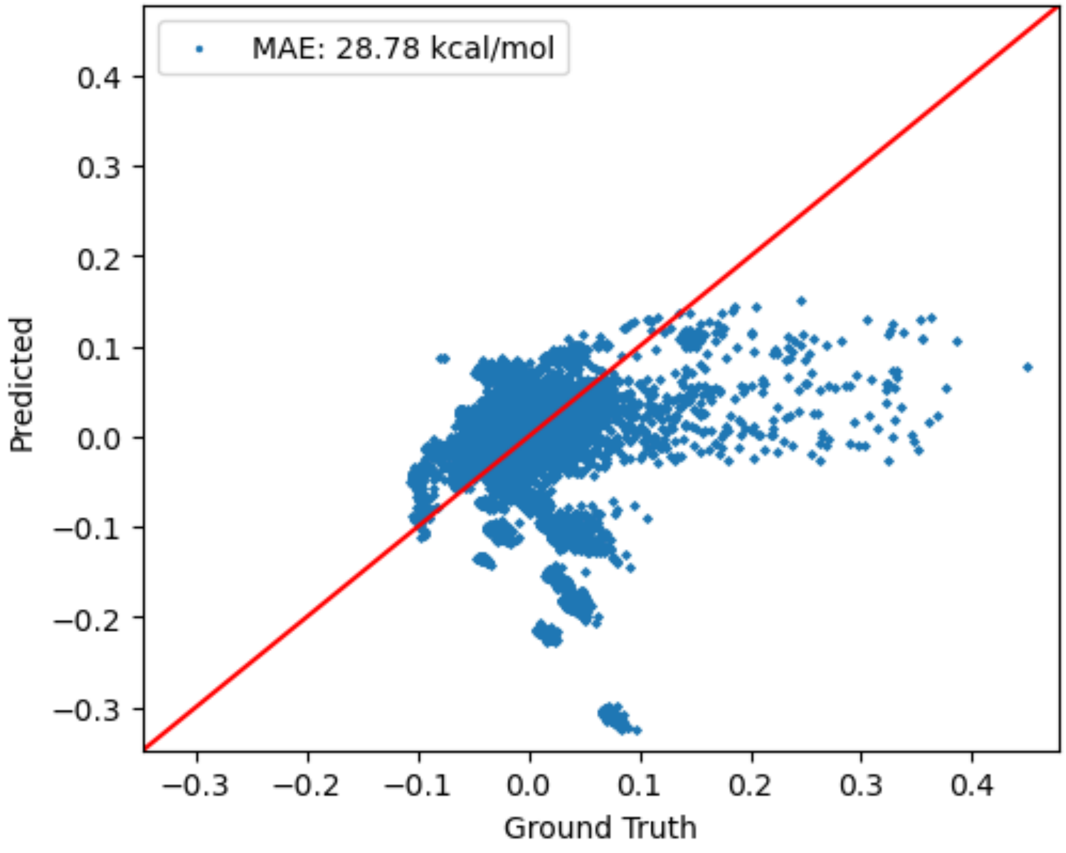
```
Sequential - Number of parameters: 197636
Initialize training data...
100%|██████████| 30/30 [05:15<00:00, 10.53s/it]
```


MAE: 28.78 kcal/mol
Predicted
Ground Truth
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
−0.3
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4


Train
Validation
Loss
# Batch
10^0
10^{-1}
10^{-2}
0
5
10
15
20
25
30

In [18]:
```
trainer.evaluate(test_data, draw_plot = True)
```

Out[18]:
```
0.005383185408368 97
```



In [19]:
```
print(train_losses)
```

```
[1.5109391065437816, 0.5500195810874008, 0.2331469871181487, 0.1459520590001
274, 0.11423158201673402, 0.09482943795281365, 0.0804987498352487, 0.0696012
8407505019, 0.06115456678750528, 0.05439721283410198, 0.048772662073493796,
0.04390613837408042, 0.039564907185506995, 0.035615733834595716, 0.031988203
731551416, 0.02864782305148718, 0.025578042204748432, 0.02276968319424918,
0.020215203202925903, 0.017906103204565784, 0.01583196588893969, 0.013980424
235496773, 0.012337452546964849, 0.010887857790499698, 0.00961575704842344,
0.008504947504170511, 0.007539339923724219 4, 0.006703351922989068, 0.0059820
55371318673, 0.005361442608532155]
```

This led to a worse performance than all the previous iterations. The loss is 0.005361442608532155 and the MAE is a very high 28.78 kcal/mol.

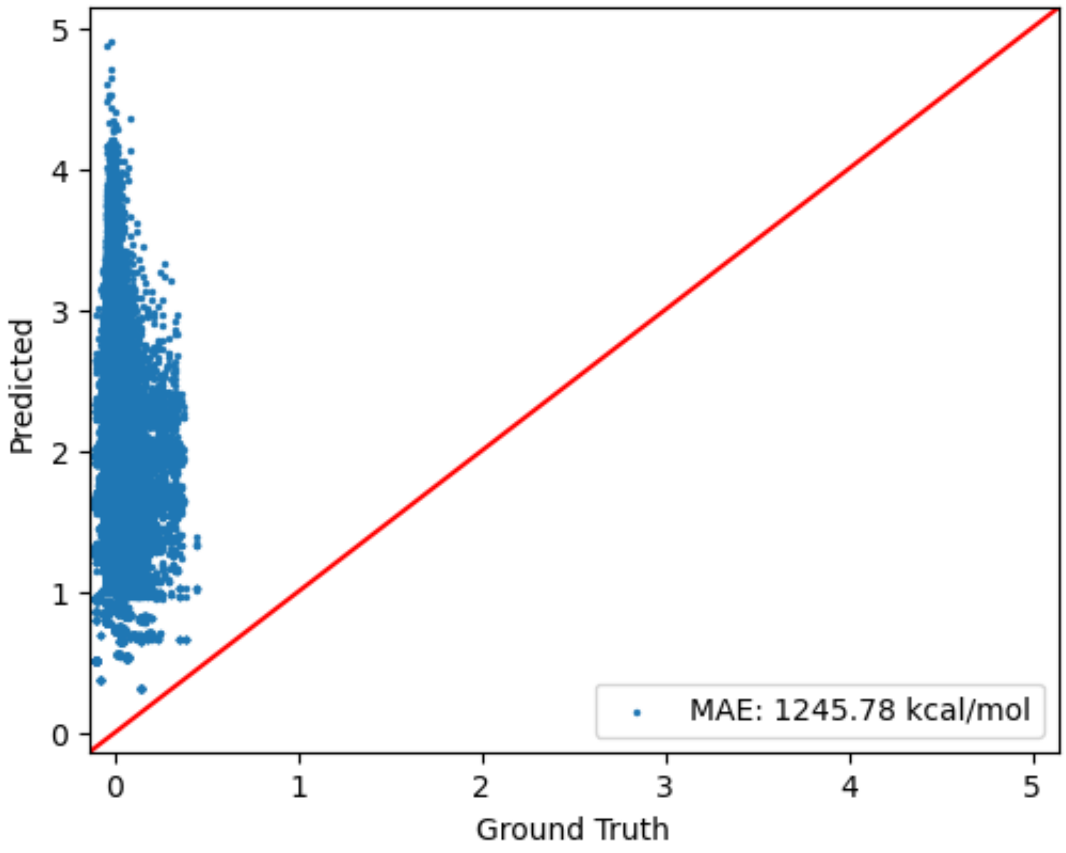
Iteration 5

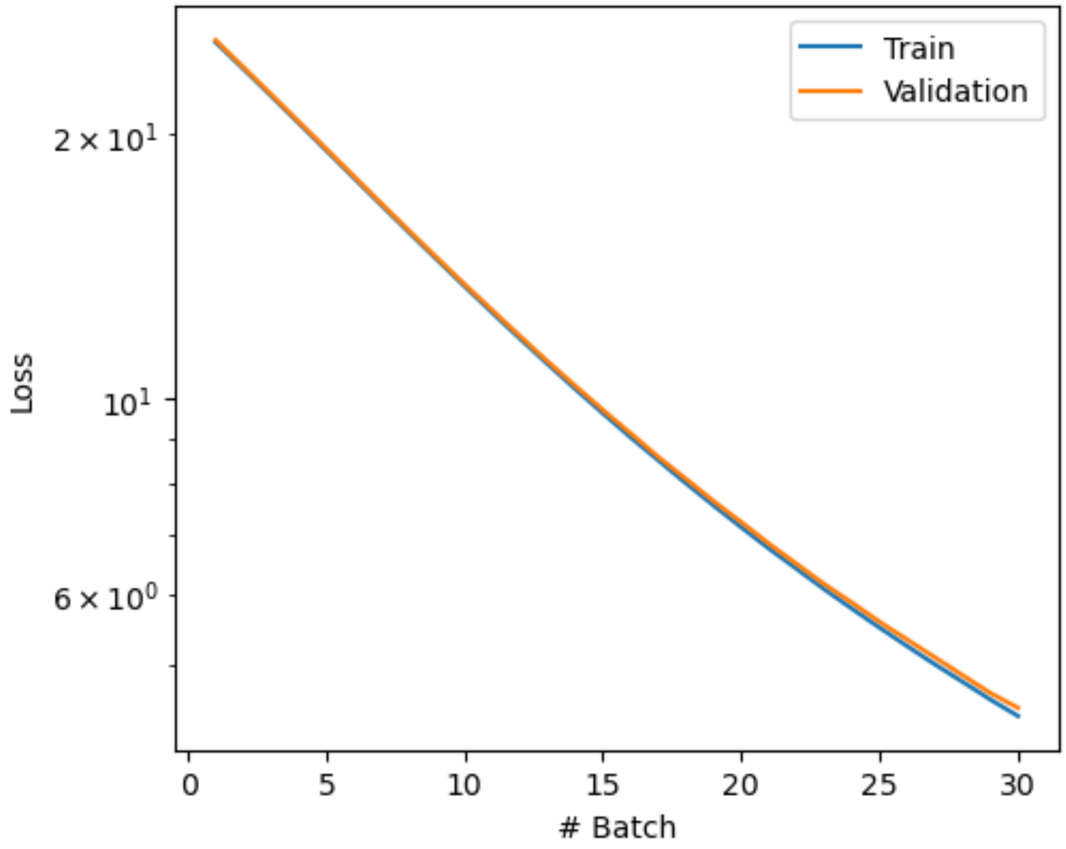
Here I add dropout with the Sigmoid activation function.

In [20]:
```
# Add Dropout
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 128),
            nn.Dropout(p=0.15),
            nn.Sigmoid(),
            nn.Linear(128, 1),
            nn.Dropout(p=0.15),
            nn.Sigmoid(),
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torch.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [21]:
```
model = model

trainer = ANITrainer(model, learning_rate=1e-5, batch_size = 8192, epoch = 3

train_losses, val_losses = trainer.train(train_data, val_data)
```

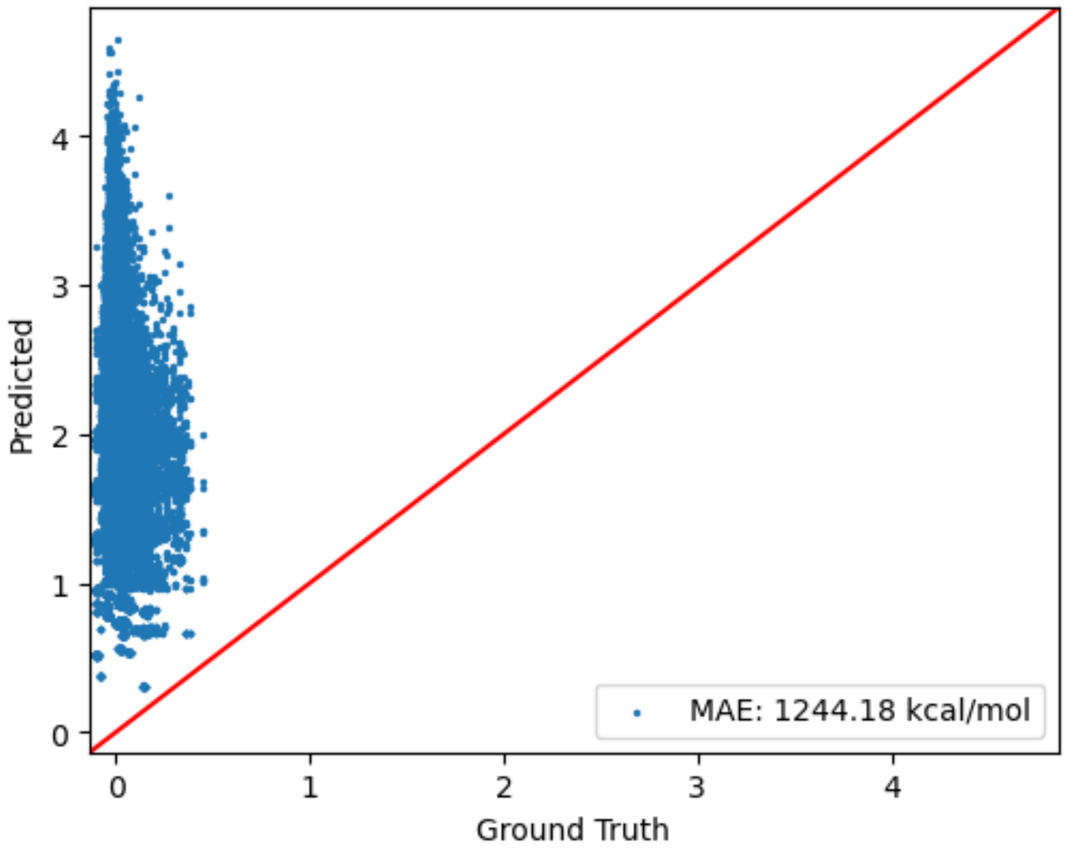
```
Sequential - Number of parameters: 197636
Initialize training data...
100%|██████████| 30/30 [04:55<00:00,  9.85s/it]
```


Predicted
Ground Truth
MAE: 1245.78 kcal/mol
0
1
2
3
4
5


Loss
# Batch
Train
Validation
2×10^1
10^1
6×10^0
0
5
10
15
20
25
30

In [22]:
```
trainer.evaluate(test_data, draw_plot = True)
```

Out[22]:
```
4.452102335629386
```



In [23]:
```
print(train_losses)
```

```
[25.42728441695278, 23.7217000573818, 22.106758819508894, 20.58712591213645
7, 19.163246333882157, 17.8357531841696, 16.600765391986602, 15.457164777947
526, 14.405716801323448, 13.43582456236555, 12.53967674584036, 11.7194286971
87189, 10.966857420888148, 10.273054157884143, 9.63960918208587, 9.054474303
075532, 8.526406179845244, 8.029856606249867, 7.575496110684058, 7.157020076
723713, 6.769853723063323, 6.419699803022335, 6.087143596358469, 5.785909187
165259, 5.504668085305071, 5.244672303925321, 5.001379956716937, 4.778309161
511738, 4.56298850804464, 4.369976060625383]
```

Similar to the last iteration, iteration 5 did not reduce the loss and performed worse than the previous iterations. The loss was 4.369976060625383 and the MAE is the highest it has been, 1244.18 kcal/mol. Evidently, dropout is not an effective regularization technique for this dataset.

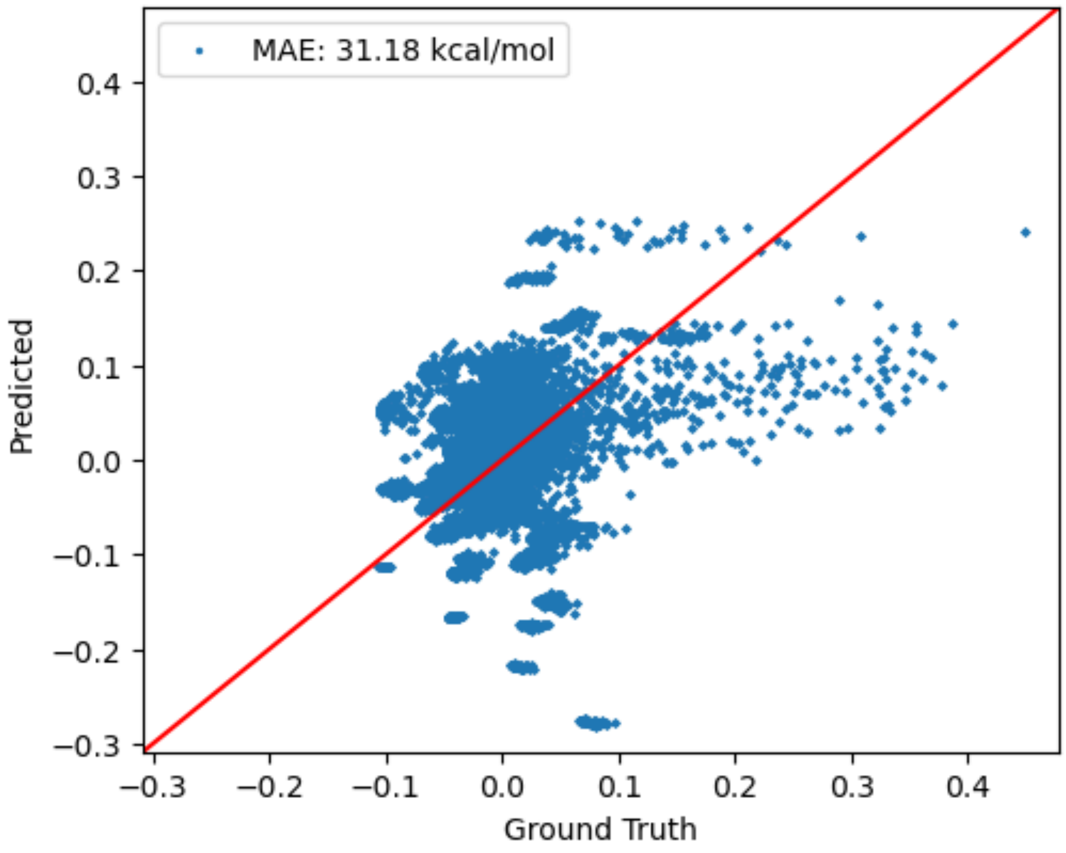
Iteration 6

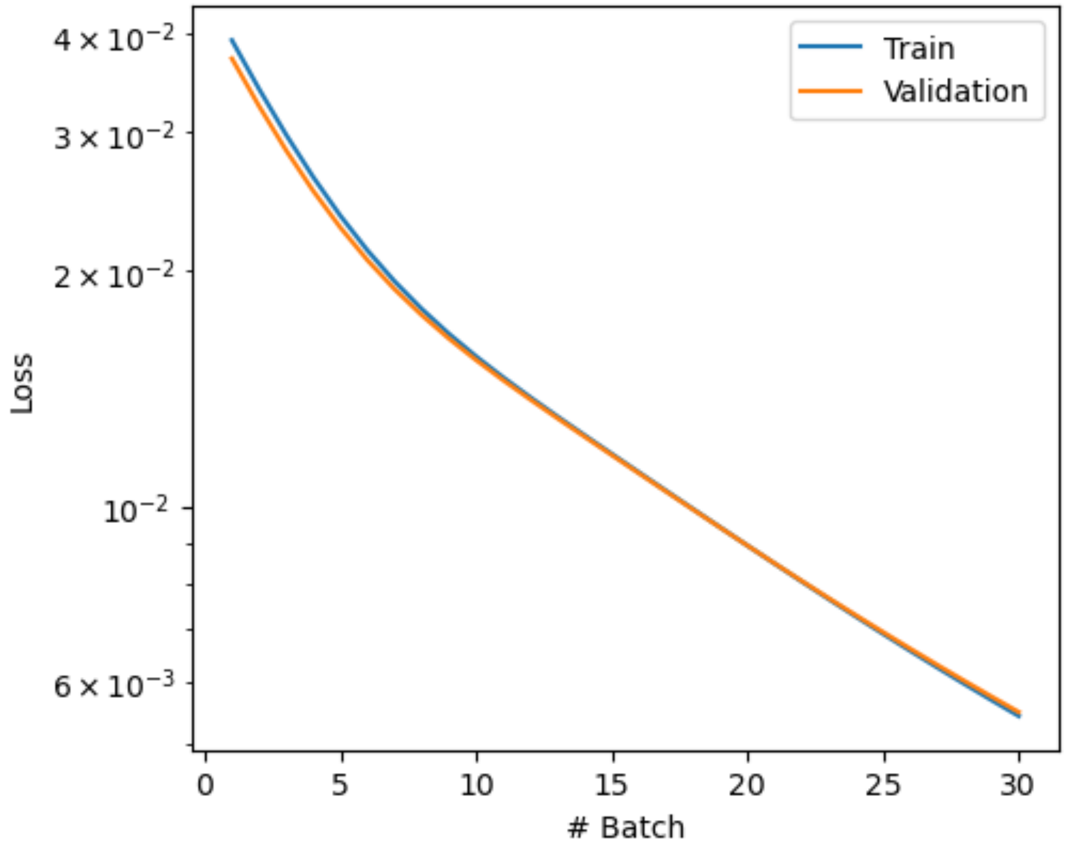
Adding an additional hidden layer and decreasing the batch size and decreasing the learning rate

In [24]:
```
# change to 2 hidden layers
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 128),
            nn.ReLU(),
            nn.Linear(128, 64),
            nn.ReLU(),
            nn.Linear(64, 1)
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torch.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [25]:
```
model = model

trainer = ANITrainer(model, learning_rate=1e-6, batch_size = 512, epoch = 30

train_losses, val_losses = trainer.train(train_data, val_data)
```

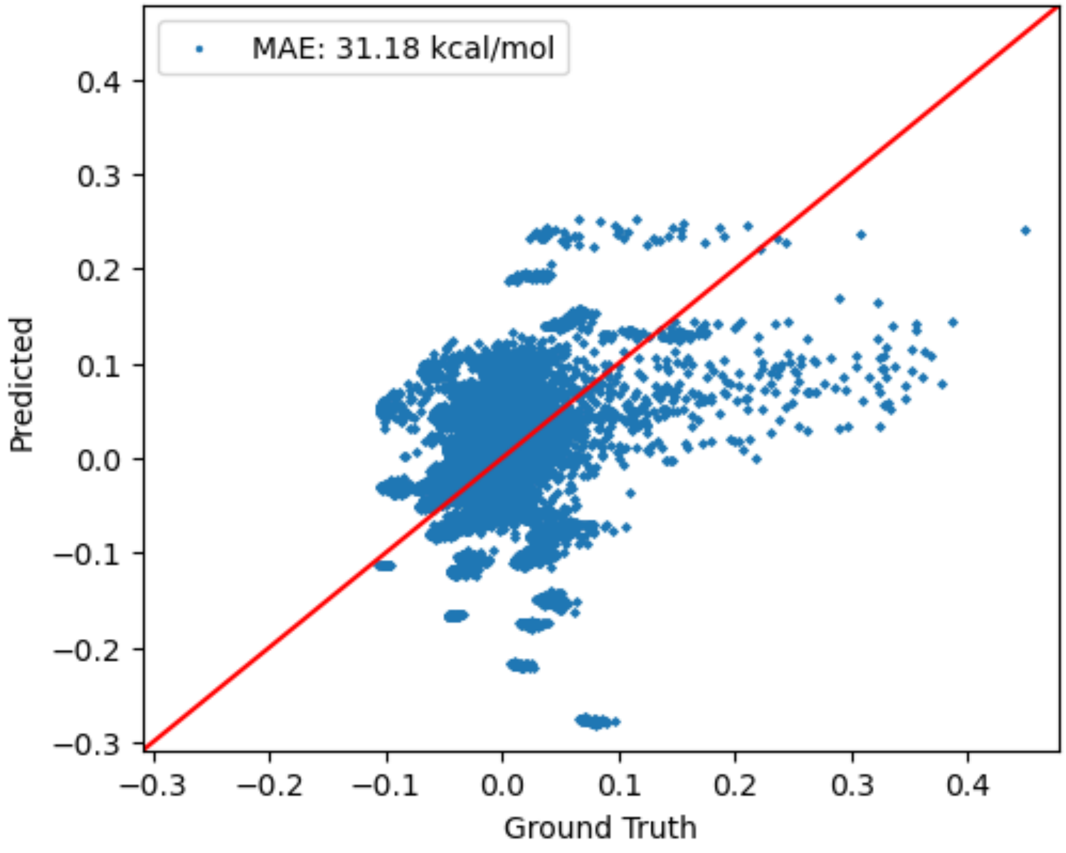
```
Sequential - Number of parameters: 230404
Initialize training data...
100%|██████████| 30/30 [05:12<00:00, 10.42s/it]
```


MAE: 31.18 kcal/mol
Predicted
Ground Truth
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
−0.3
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4


Train
Validation
Loss
# Batch
4×10^{-2}
3×10^{-2}
2×10^{-2}
10^{-2}
6×10^{-3}
0
5
10
15
20
25
30

```
In [26]: trainer.evaluate(test_data, draw_plot = True)
```

```
Out[26]: 0.005478806803251806
```



```
In [27]: print(train_losses)
```

```
[0.03929618941770233, 0.034070429020977566, 0.02978522476788199, 0.026300331
83955821, 0.02348309789126103, 0.021210439898901142, 0.019370547304545196,
0.017865402058884282, 0.01661317994193476, 0.015548132281081628, 0.014619789
697872967, 0.013791077278980724, 0.013036152717752358, 0.012337521710276028,
0.011683877044643815, 0.01106817112568961, 0.010486652314335971, 0.009937363
379443571, 0.009418975679104711, 0.008930188727469417, 0.008469817711170233,
0.008036897714337686, 0.007630460965456753, 0.007249356522645049, 0.00689223
2608928757, 0.006557624200998794, 0.006244065058841623, 0.00595021616373908
5, 0.005674777854223976, 0.005416390709110152]
```

From iteration 6, we can see that that the loss only decreased to 0.005416390709110152 which is still not as optimal as iteraiton 1. The MAE of 31.18 kcal/mol is again not optimal.

Conclusions

From 6 iterations of modifying the atomic net architecture and tuning the hyperparameters, I can see that what helped optimize the loss most was the learning rate. Decreasing the learning rate helped stabilize oscillation in the loss functions that were seen when the learning rate was 1e-3. Furthermore, decreasing the learning rate to 1e-5 helped decrease the overall loss to its lowest point of 1.1774181918935158e-05 and led to a test/val MAE of 1.30 kcal/mol.

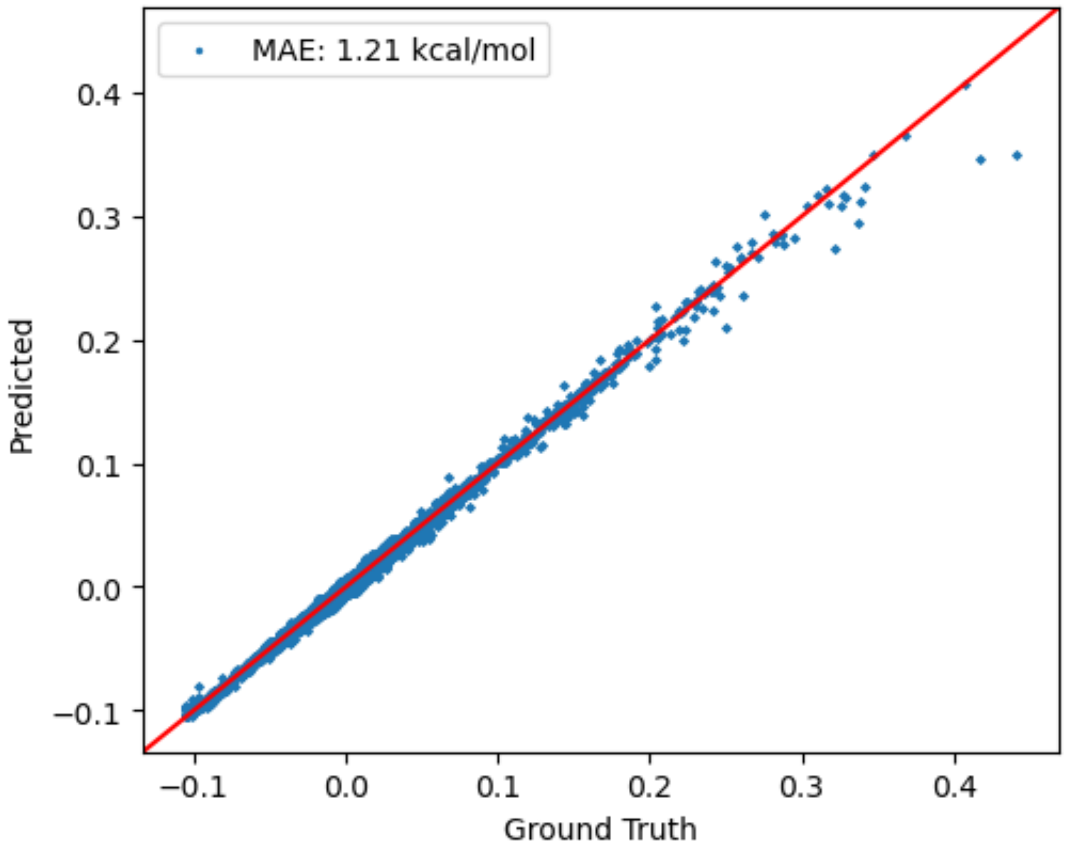
Checkpoint 4

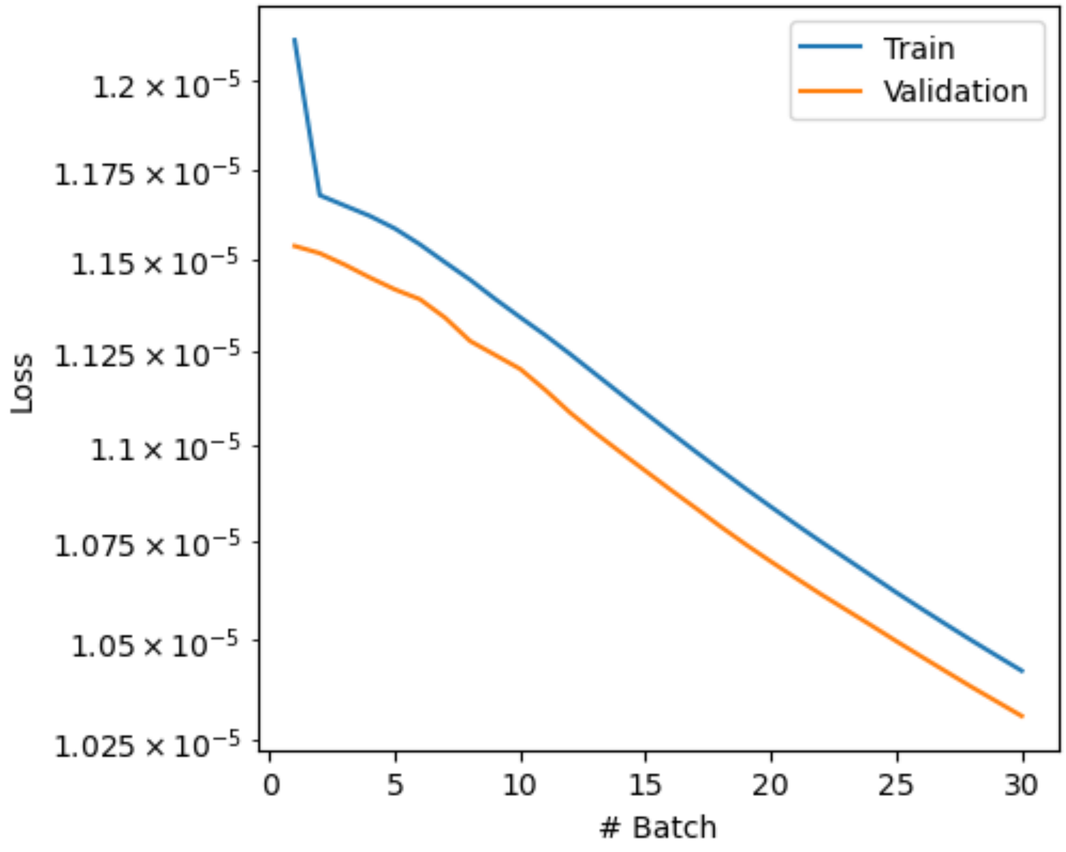
The best model architecture was from Iteration 1, having a learning rate of 1e-5, batch size of 8192, l2 of 1e-5 and 30 epochs.

In [21]:
```
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [22]:
```
model = model

# tried decreasing the learning rate
trainer = ANITrainer(model, learning_rate=1e-5, batch_size = 8192, epoch = 3

train_losses, val_losses = trainer.train(train_data, val_data)
```

```
Sequential - Number of parameters: 197636
Initialize training data...
100%|██████████| 30/30 [04:47<00:00,  9.58s/it]
```


MAE: 1.21 kcal/mol
Predicted
Ground Truth
0.4
0.3
0.2
0.1
0.0
−0.1


Train
Validation
Loss
# Batch
1.2×10^{-5}
1.175×10^{-5}
1.15×10^{-5}
1.125×10^{-5}
1.1×10^{-5}
1.075×10^{-5}
1.05×10^{-5}
1.025×10^{-5}
0
5
10
15
20
25
30

```
In [ ]:
```