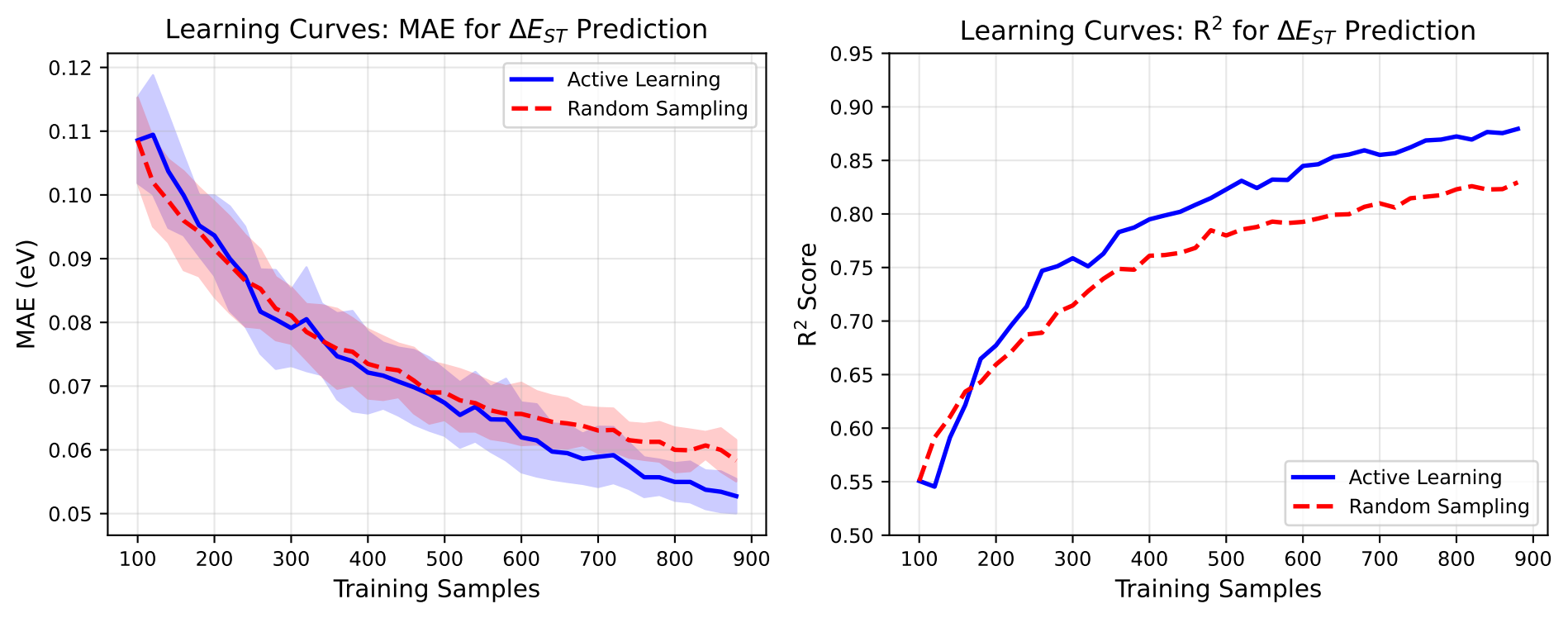
Learning Curves: MAE for ΔE_{ST} Prediction
MAE (eV)
Training Samples
Active Learning
Random Sampling
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
100
200
300
400
500
600
700
800
900
Learning Curves: R^2 for ΔE_{ST} Prediction
R^2 Score
Training Samples
Active Learning
Random Sampling
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50