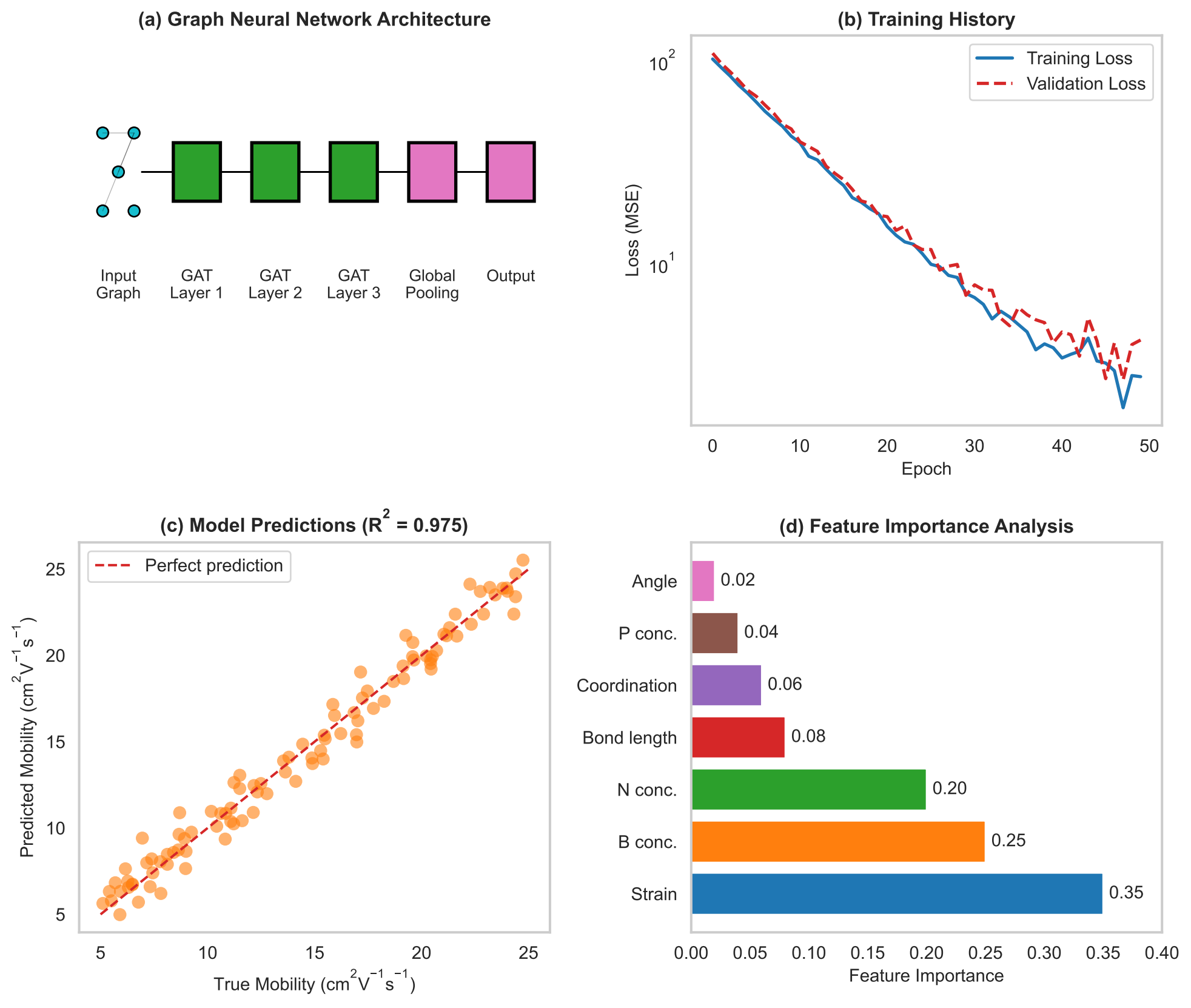
(a) Graph Neural Network Architecture
Input Graph
GAT Layer 1
GAT Layer 2
GAT Layer 3
Global Pooling
Output
(b) Training History
Training Loss
Validation Loss
Loss (MSE)
Epoch
(c) Model Predictions (R^2 = 0.975)
Perfect prediction
Predicted Mobility ($cm^2V^{-1}s^{-1}$)
True Mobility ($cm^2V^{-1}s^{-1}$)
(d) Feature Importance Analysis
Angle
P conc.
Coordination
Bond length
N conc.
B conc.
Strain
0.02
0.04
0.06
0.08
0.20
0.25
0.35
Feature Importance