Graph Neural Network Architecture for Graphullerene Property Prediction

Node Features:
• Atomic type
• Position
• Local environment

Edge Features:
• Bond type
• Distance
• Strain tensor

Attention Weights:
• $\alpha\_ij = \text{softmax}(e\_ij)$
• $e\_ij = \text{LeakyReLU}(a^T[Wh\_i||Wh\_j])$

Model Performance:
• $R^2 = 0.975$
• MAE < 0.5 cm²V⁻¹s⁻¹
• Training: 500+ DFT calculations

Input Graph
(Molecular Structure)

α_{ij}

GAT Layer 1
(128 neurons)

GAT Layer 2
(128 neurons)

GAT Layer 3
(128 neurons)

Global
Pooling

Output Layer
(Band Gap, Mobility, Formation Energy)