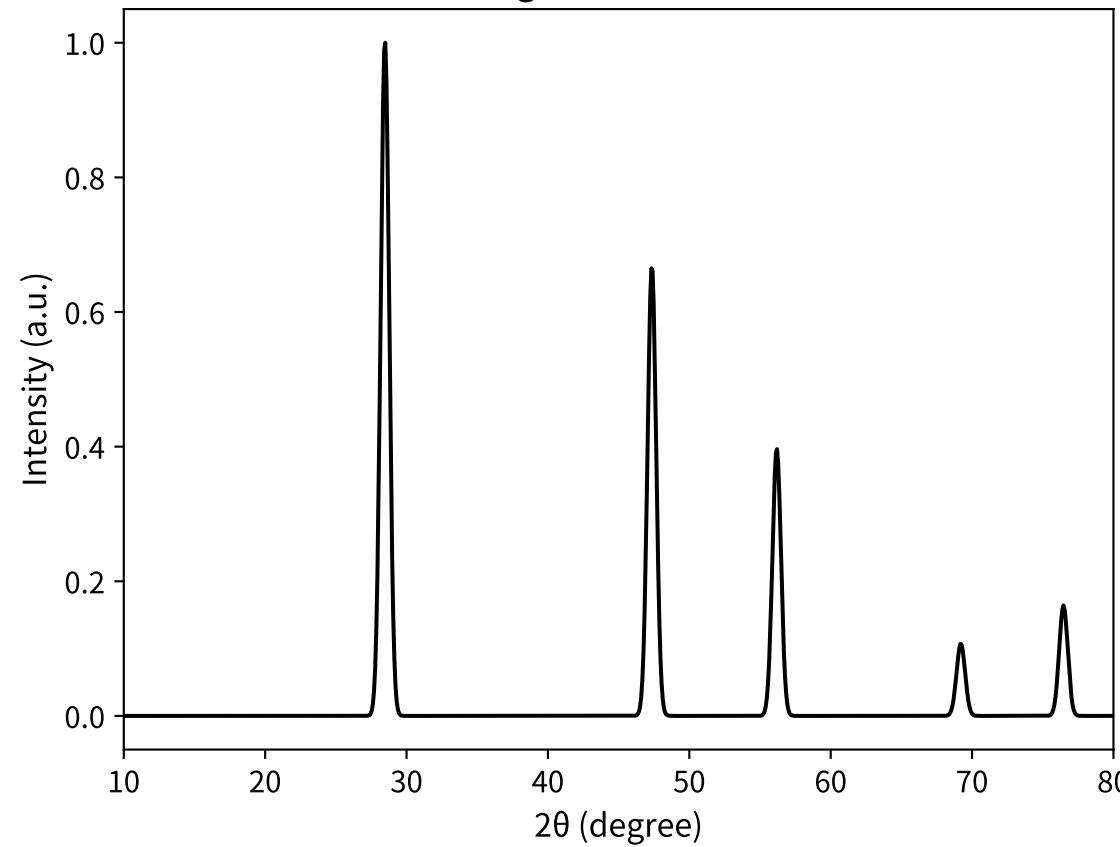
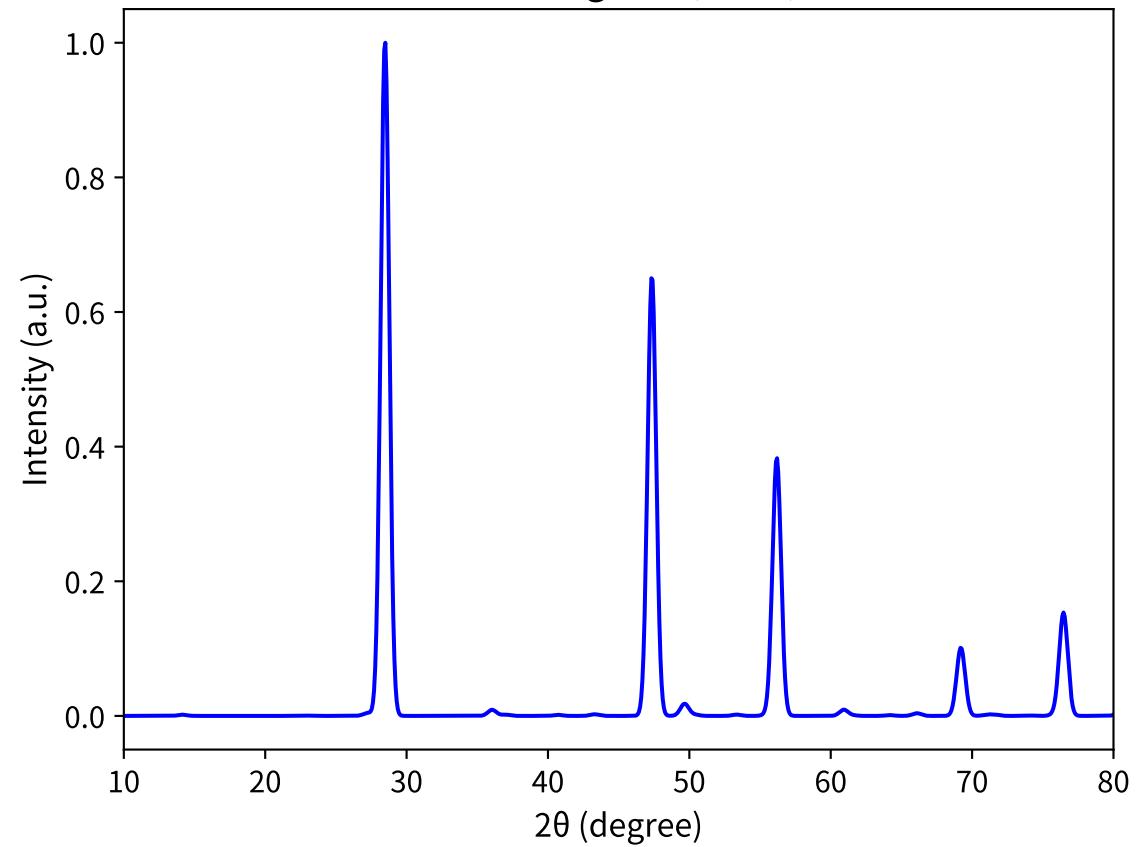


Si XRD Patterns: MD Augmentation Comparison (MACE)

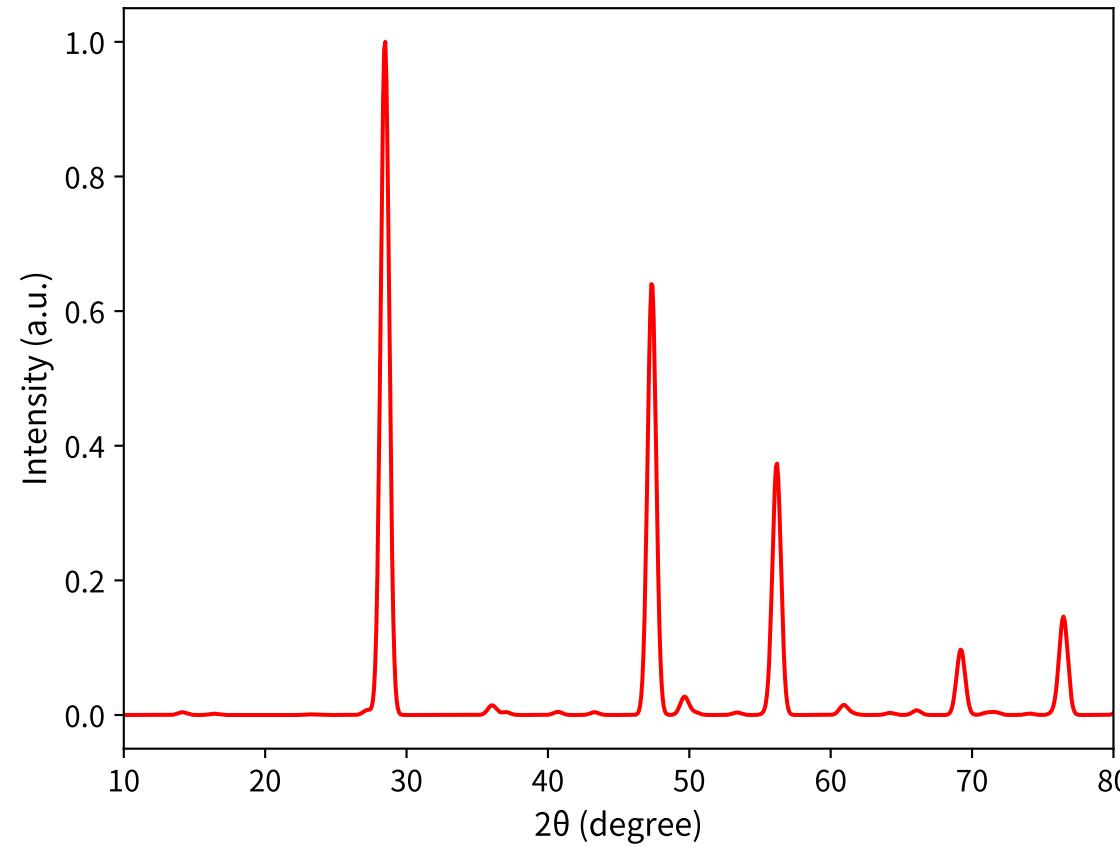
Original Structure



NVT-Langevin (300K)



NVT-Berendsen (300K)



NPT-Berendsen (300K, 1atm)

