Start: Pre-trained SCAN **Aggregate Losses** 10^{4} 10³ 10^2 Deviation (kcal/mol) 10^{1} 10⁰ 0 -10⁰ -10^{1} -10^{2} ae -10^{3} rho Total 50 150 100 200 250 300 350 400 0 **Epoch**