Start: Pre-trained SCAN **Aggregate Losses** 10⁴ 10³ 10^2 Deviation (kcal/mol) 10¹ 10⁰ 0 -10° -10^{1} -10^{2} Ε ae -10^{3} rho Total 20 40 50 60 80 10 30 70 **Epoch**