Start: Pre-trained SCAN E/Rho Losses 60 50 Deviation (kcal/mol) Energy Loss Value 40 C 30 Na 0 20 10 0 0 50 100 150 200 250 300 350 400 C2H2 0.0030 CH CHN 0.0025 CO Deviation (e) Rho Loss Value CO₂ 0.0020 F2 FLi Н 0.0015 H2 HLi 0.0010 Li NO 0.0005 Na2 0.0000 200 0 50 100 150 250 300 350 400 **Epoch**