MSE_o 0.0005 5 3 46 32 49 22 31 41 16 19 18 1 30 23 7 48 21 15 4 9 2 0 Force prediction error $(kcal/molA)^2$ 0.0004 Mean 40 37 42 43 44 35 38 20 47 28 25 10 39 0.0003 13 6 0.0002 27 36 12 0.0001 26 0.0000 10 20 30 40 50 Cluster index