Ewald sum results ($\sigma = 5 \cdot 10^{-11}$, $n_{cut} = 5$) Electrostatic energy Madelung constant -3443.95 -1.74756 -3444.1 -1.74764 E_{ewald} in kJ/mol $\stackrel{p}{\mathcal{U}}_{m}$ -1.74772 -3444.26 -1.7478 -3444.41 -3444.56 -1.74787 20 10 15 10 15 20 k_{cut} k_{cut} Execution time Memory usage 70 60 8 50 6 *m* in MiB t_{run} 30 20 2 10 0 0 10 15 20 10 15 20 k_{cut} k_{cut}