Total number of microstates along separation coordinate 3.5×10^7 8.3×10^9 2.0×10^{10} 5.3×10^8 2.6×10^9 048 -5 $\Delta A~(kJ/mol)$ 36 time (h) -1024 -1512 -200 8 10 2 8 10 6 4 6 4 ξ (Å) grid factors 0 -1020 $-T\Delta S$ (kJ/mol) $\Delta E~(kJ/mol)$ -2010 -30-40010 6 8 10 446 8 ξ (Å) ξ (Å)