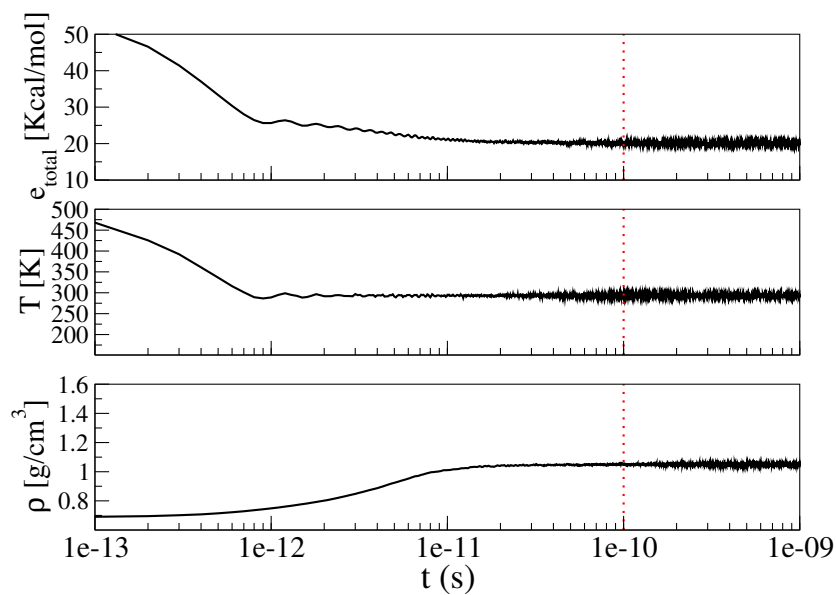


Supplementary Material II



Plot of the total energy per molecule (top), temperature (middle) and density (bottom) for the equilibration run of one system of 1000 Hexamethylene diisocyanate molecules (HDI) in NPT ensemble, held at a temperature of 293.15 K and at a pressure of 1 atm. The simulation starts from the final configuration obtained from the scale-and-run stage. Red dashed line indicates the point at which equilibrium is reached.