

**Supplementary material: Determining the phase diagram of
water from direct coexistence simulations: the phase diagram of
the TIP4P/2005 model revisited**

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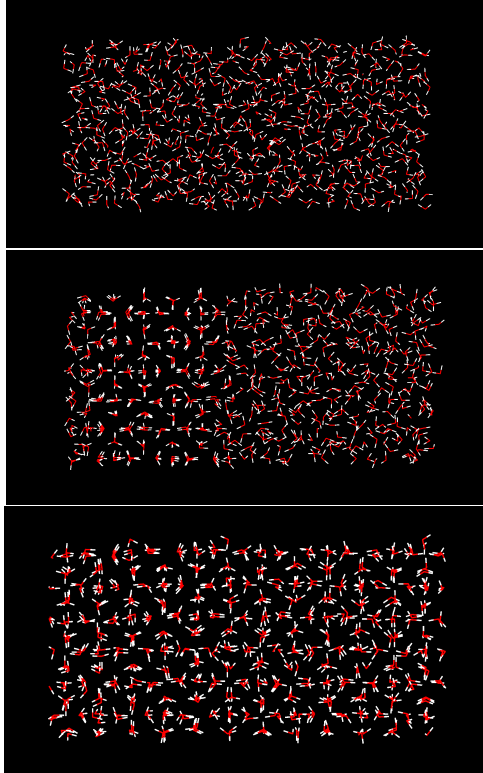


FIG. 1. Snapshots of TIP4P/2005 model for the system ice VI-liquid water at 12000 bar. The initial configuration is shown in the middle panel. The upper panel shows the final configuration of a run at 270 K and the final configuration at 266 K is shown at the bottom.

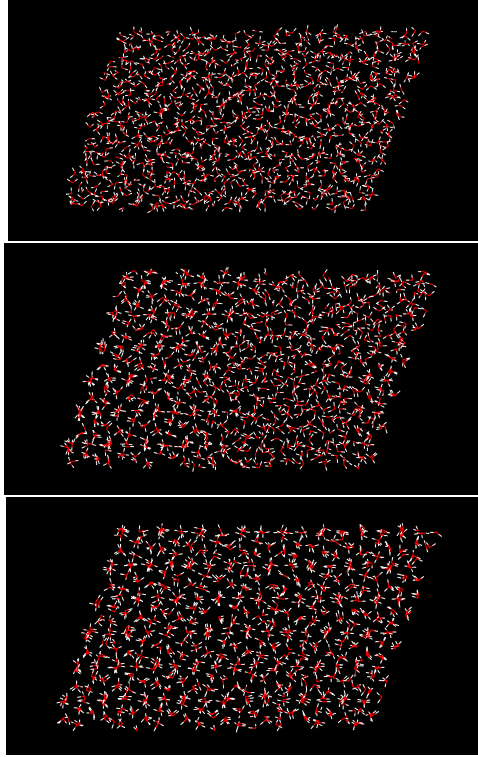


FIG. 2. Snapshots of the ice V-liquid water system at 7000 bar for TIP4P/2005 model. The initial configuration is shown in the middle panel. The upper panel shows the final configuration of a run at 243 K and the final configuration at 237 K is shown at the bottom.

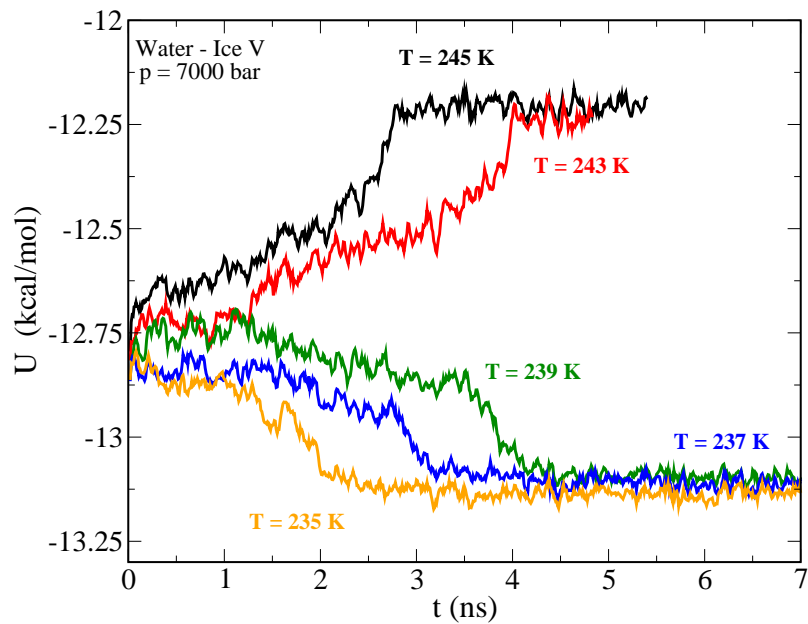


FIG. 3. Evolution of the potential energy as a function of time in NpT runs for the system formed by ice V and liquid TIP4P/2005 water at 7000 bar.

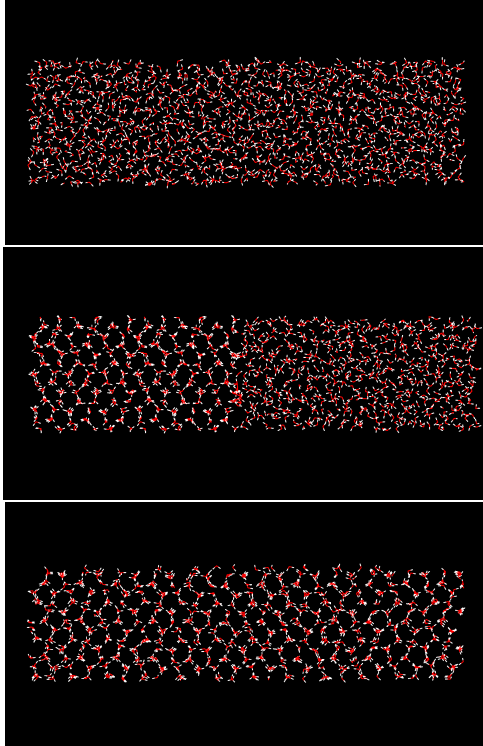


FIG. 4. Snapshots of the ice III-liquid water system at 3500 bar for TIP4P/2005 model. The initial configuration is shown in the middle panel. The upper panel shows the final configuration of a run at 250 K and the final configuration at 234 K is shown at the bottom.

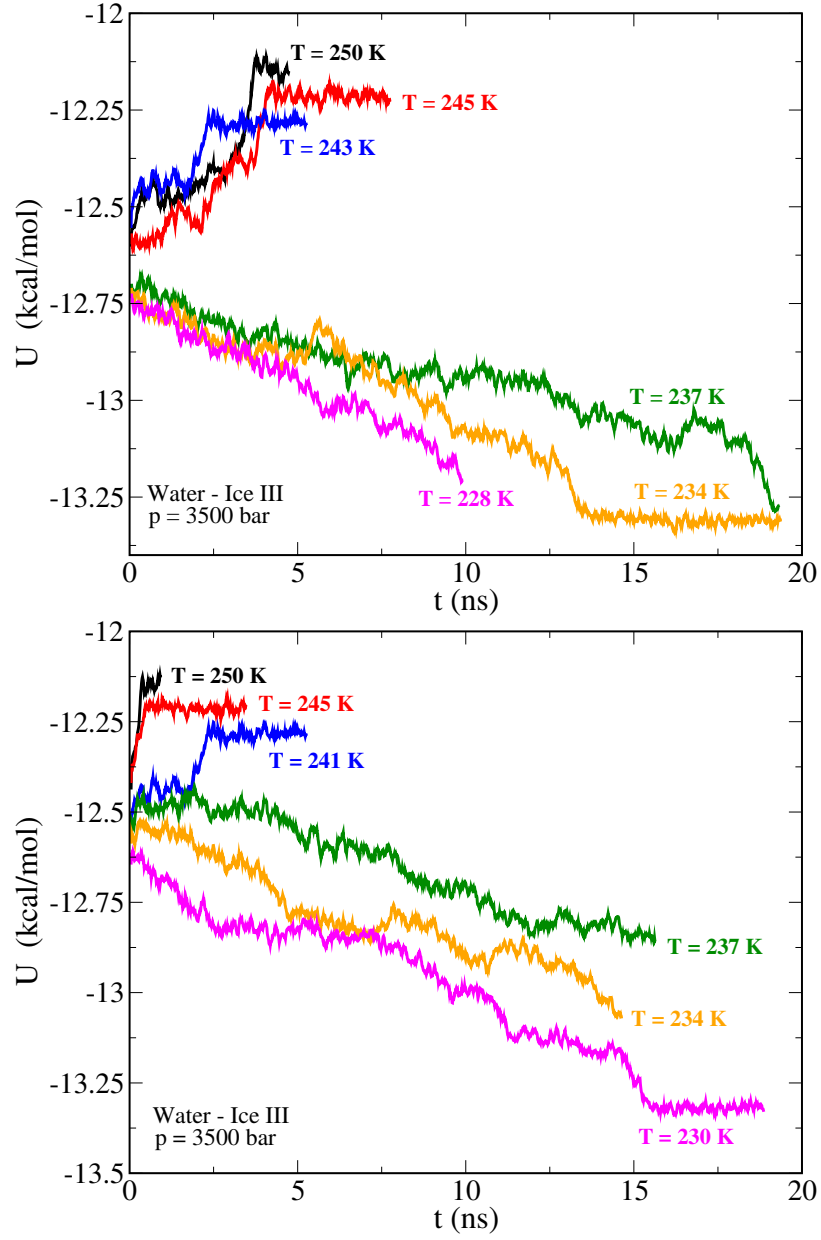


FIG. 5. Evolution of the potential energy as a function of time for the NpT runs for TIP4P/2005 at 3500 bar for the system formed by ice III and liquid water for two different initial configurations of ice III.