CNS Assignment 6

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1 Free Energy Surface for the association process of Na⁺ and Cl⁻ using Umbrella Sampling Simulations

Umbrella Sampling method was used to reach all the parts of the free energy surface. On obtaining the Relative probability distribution from each of the bins we get the outputs of the probabilities of the different bond lengths. The histograms the plotted from this data are analysed by WHAM if they have overlap.

using the tool from Grossfield Labs.
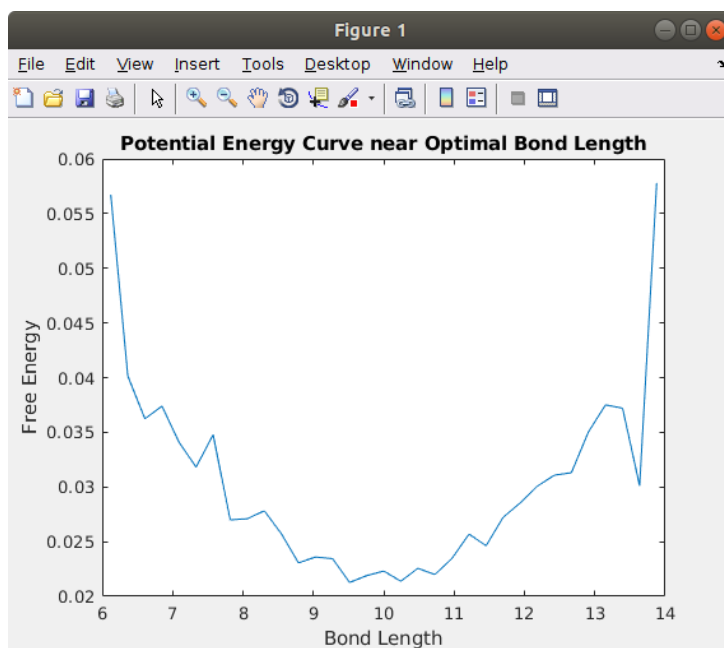
1.1 Free Energy Surface

Figure 1: 2BAW

The bond length comes out to be approximately 9.5, as the lowest minima is there.

2 Solvation free energy of methanol and n-butanol

Thermodynamic Integration is used to fine the Solvation free energy of methanol and n-butanol.

The TI output file gives the average VDW and Electrostatic Energies.

The Enrergy values for methanol are always higher than butanol, hence methanol is more soluble in water.