2018113003

Assignment 6

18th September 2018

QUESTION

Calculate the free energy surface for the association process of Na+ and Cl- using umbrella sampling simulations.

Umbrella Sampling

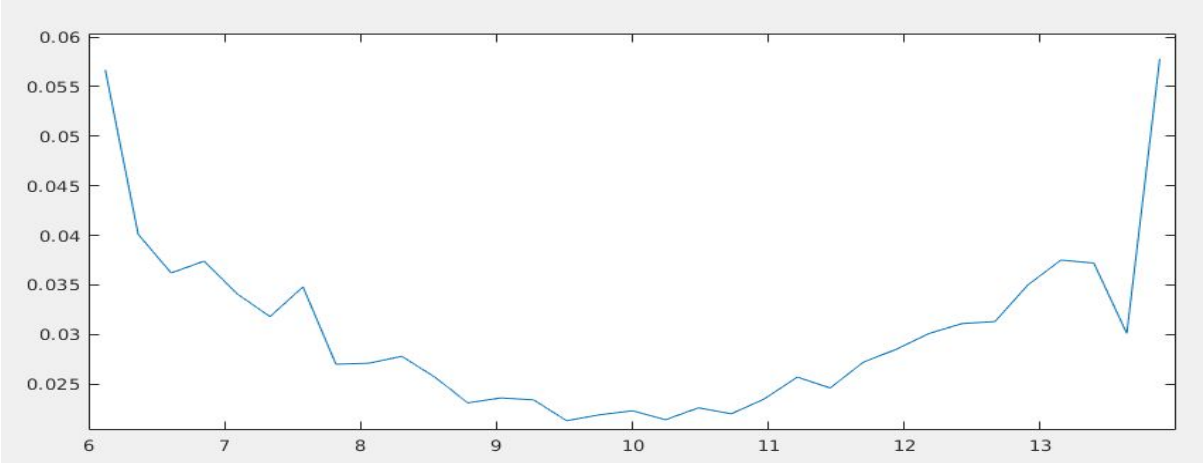
Umbrella sampling is done to find energy of a molecule beyond its minima. By default, NAMD cannot stimulate past a minima, thus not able to calculate data for different reaction coordinates.

Here Umbrella Sampling comes in useful. Umbrella Sampling creates a potential barrier(in the form of a parabola) centered at a coordinate. The barrier does not allow the molecule to go beyond the vicinity of the centre, thus forcing it to calculate energy of the reaction coordinates which were previously not computed by NAMD.

WHAM

Using an external potential distorts the original information due to there being an extra force field. To change the distorted graph to the original graph, a WHAM analysis is performed on it which computes the correct values from the distorted ones feeded to it.

RESULT



ANALYSIS

As it can be seen from the ΔG vs bond distance graph, the minima of the graph is achieved at 9.5 A. It can be concluded from the following data that the bond distance of 9.5 A is the most stable distance for the following molecule.

It can also be seen that the farther away from 9.5 A we go, higher the value of ΔG gets, thus signifying the instability of the particular bond lengths.

CONCLUSION

Thus it can be concluded from the following experiment that the optimum distance between Na+ and Cl- is 9.5 A.

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QUESTION

Calculate the solvation free energy of Methanol and Butanol.

THERMODYNAMIC INTEGRATION

Thermodynamic integration is a process in which the system starts with one molecule and vanishes it till the end of the stimulation and replacing it with other molecule. This process can be utilised in the following experiment starting with Methanol and ending with Butanol to find the solvation free energy.

RESULT

The data output contains Average electrostatic and Van der Waal Potential which are changing over the simulation. We can take the following data and plot out the results.

THEORY

The result graph is the integration of a partial derivative of Energy, the hamiltonian operator with respect to the vanishing coordinate λ.

$$\Delta A = \int_0^1 \langle \frac{\partial H(x, p_x; \lambda)}{\partial \lambda} \rangle \, d\lambda$$

$$\frac{\partial H(x, p_x; \lambda)}{\partial \lambda}$$

The output should be the result of the first equation(The integral), whereas the data we get is the second formulae. So in order to get the output, integrate the data with respect to λ.

ISSUE

We faced an issue while calculating the integral and thus getting the output desired. The perl script which calculates the integral is not accepting our input file as a valid input and thus giving us an error.

VALIDATION OF ANSWER

Our answer can be validated as the value of ΔG of Methanol is higher than that of Butanol by looking at the derivatives of both of them. The values of Average Electronic Repulsion are 135 of Methanol to 110 of Butanol thus confirming that Methanol is more soluble in water than Butanol.

CONCLUSION

It can be concluded that Methanol is more soluble in water than Butanol.