COURSE PROJECT CHM-695

MOLECULAR SIMULATION OF WATER MOLECULE

SUBMITTED BY –

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14611

Creating our own Empirical force field –

Procedure-

First we have to find optimum value of bond length and bond angle. For that we have to write opt after force field name.

Optimum bond angel = 105.4974

Optimum bond length = 0.9473 A

Now We have to calculate Ktheta, Kr as well as x0 ans theta0 from fitting.

For that we're going to take 20 points close to the equilibrium and find potential energy corresponding to each point and then fit a quadratic curve to mimic the potential calculated from quantum mechanics calculation.

I have written a script to do that, Link to scripts are given below.
https://github.com/satendrapandeymp/nnair/tree/master/Project1/Creating_input_files

Values after fitting Curve –

Ktheta = 5.86762e-05

Theta0 = 105.665

Kr = 4.87632

X0 = .949101

Now we have to turn it into Hartree units "Atomic Units".

We are also going to use values of sigma and epsilon from TIP3 forcefield.

Running Simulations –

Now we have to use molden to create a .mole2 file of water.

Then create 'water.frcmod' file and then put that data obtained by fitting into 'water.frcmod' file.

Now we have to run sander to start simulation.

This step is going to do 100,000 iterations and take nearly 1 hour.

Now we have to create a .mol2 file for dimer and trimer and We have to repeat similar steps.

Analysing Data –

After simulations are done, we have to make a directory “Analyze” and get into that directory.

Then use process_mdout.perl script with .out file to get summry of density and different other properties.

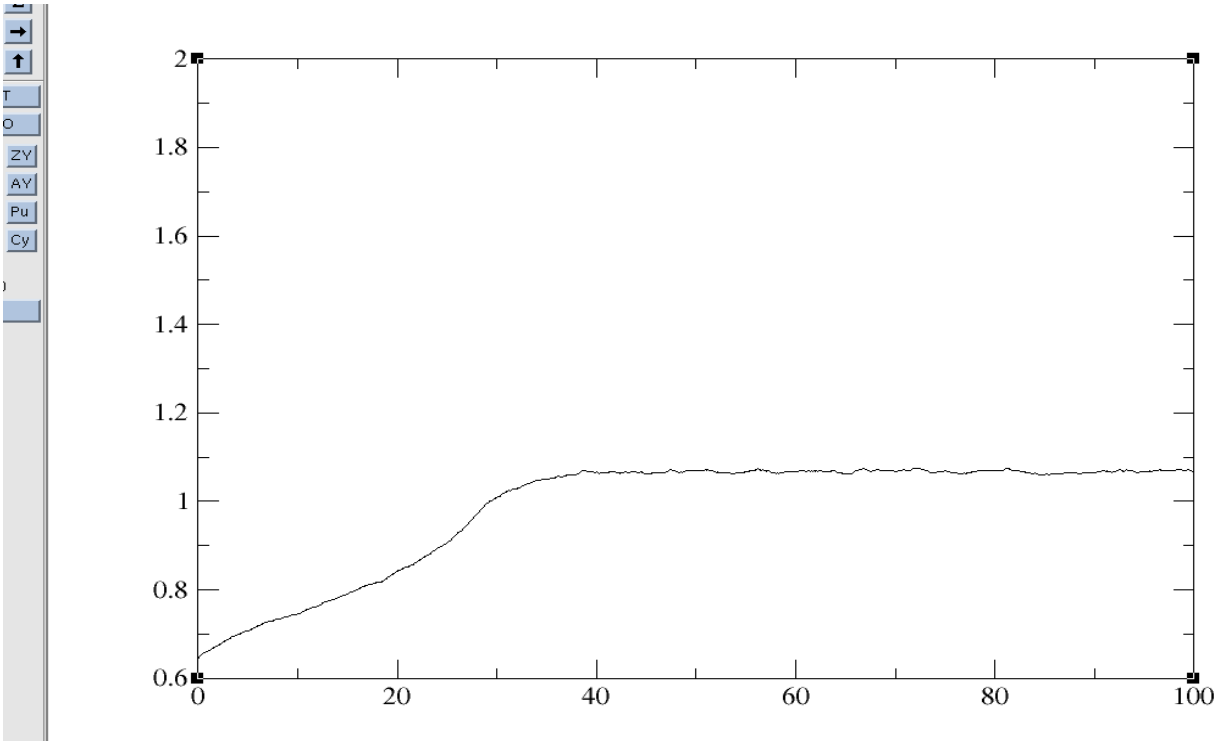
We can plot that summary using xmgrace by command “xmgrace filename”.

We are also going to use VMD with ‘.prmtop’ and ‘.rst’ file.

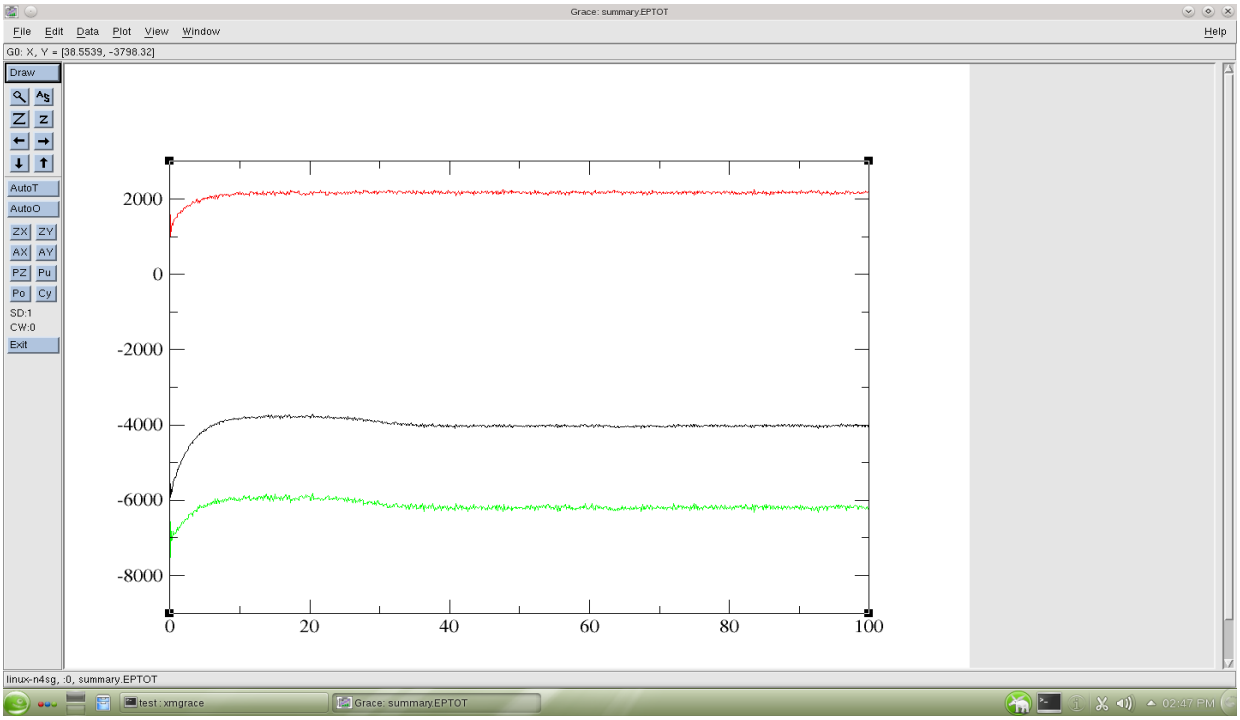
Now we can get min distance, angle as well as radial distributions of two atoms using VMD.

Results –

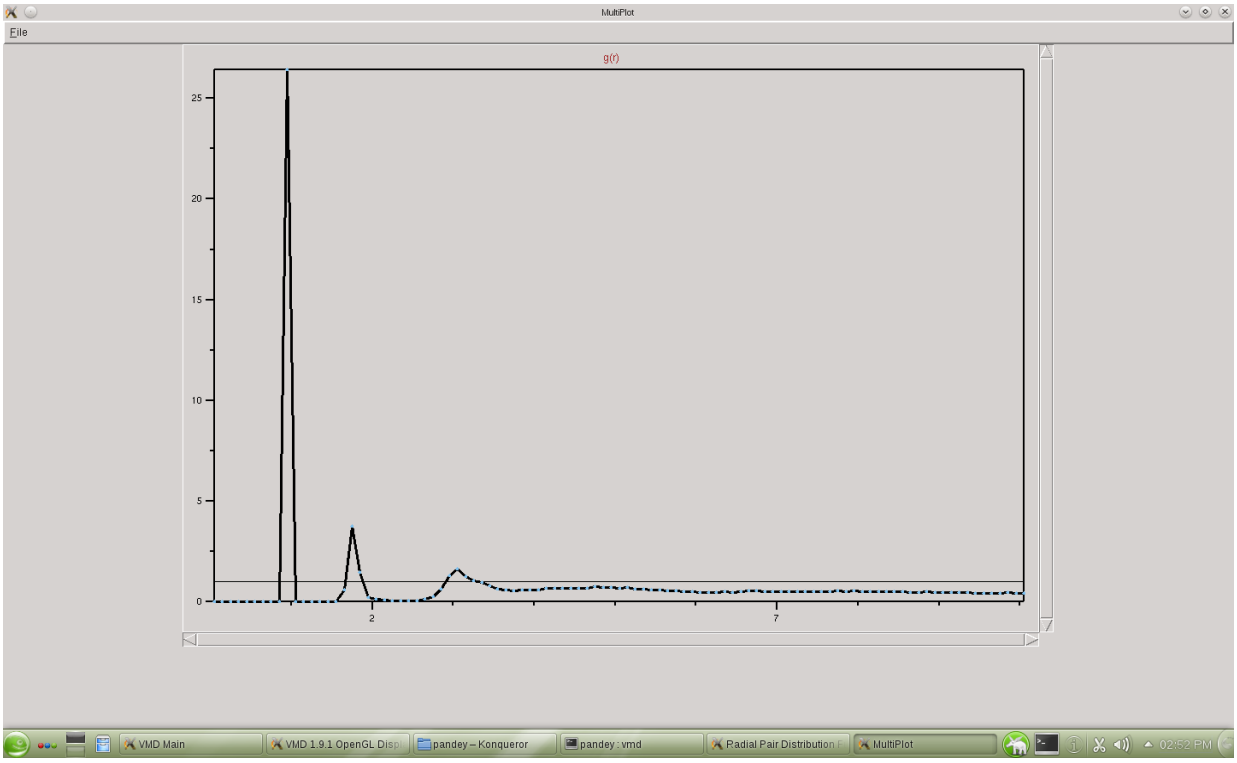
Density of Bulk Water –



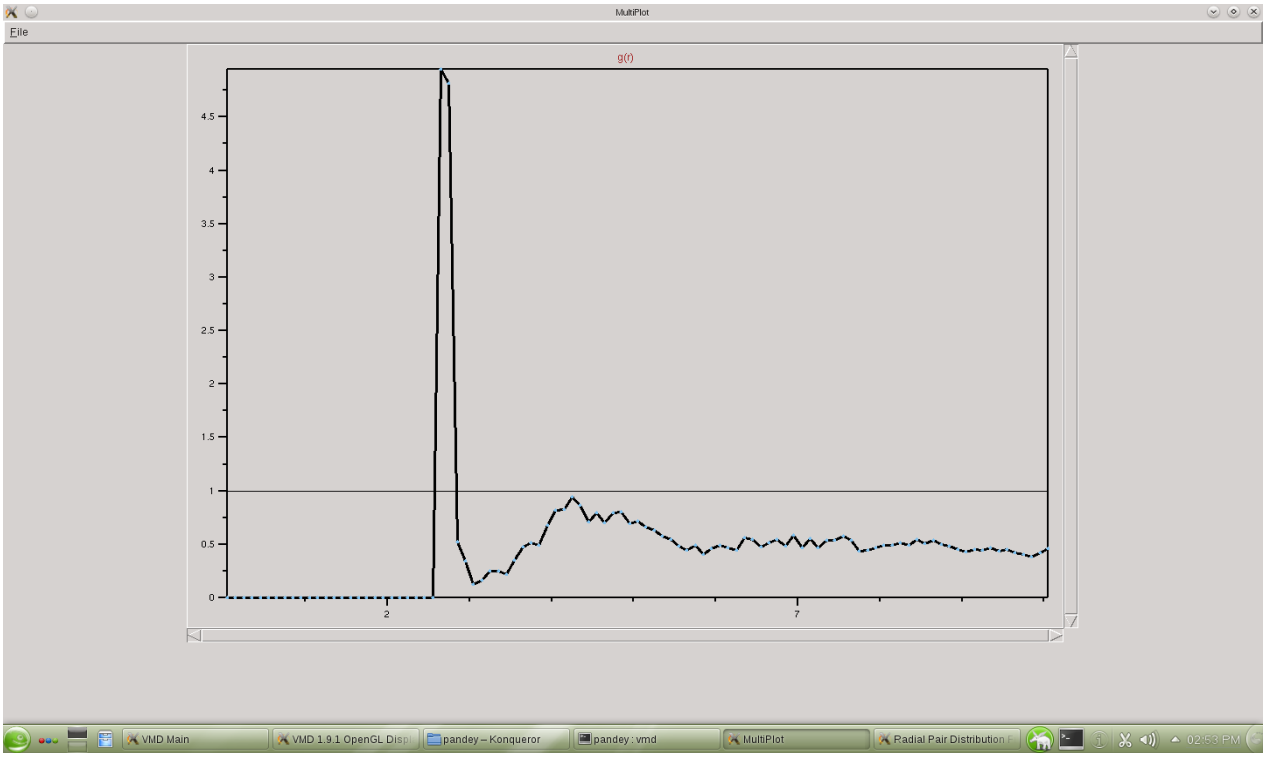
Energy of Bulk Water –



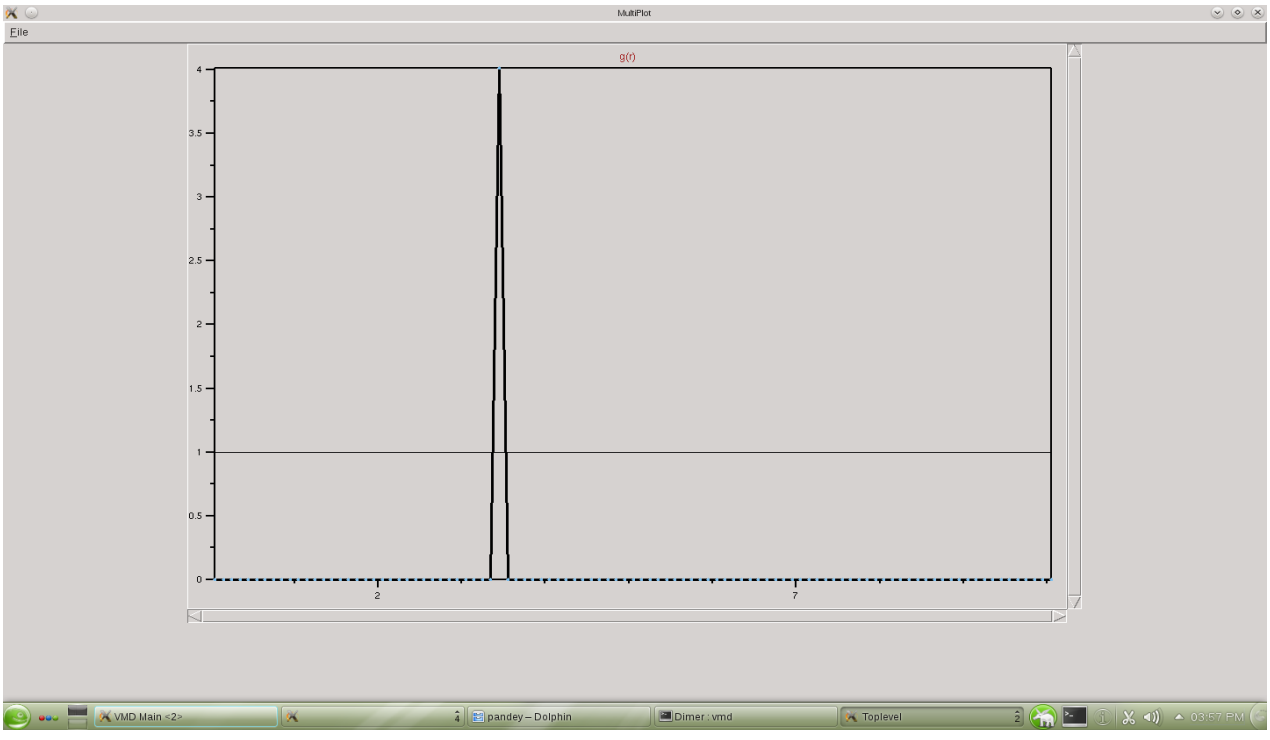
Radial Dist “O-H” –



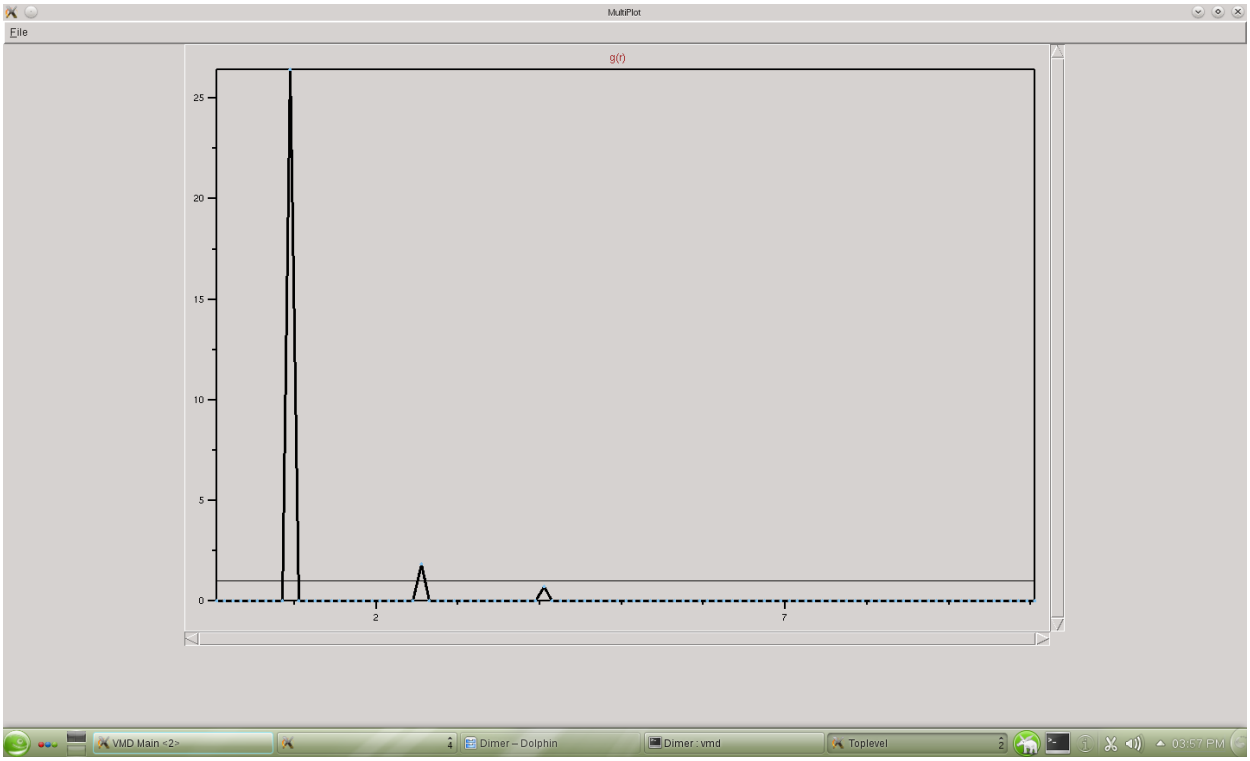
Radial Dist “O-O” –



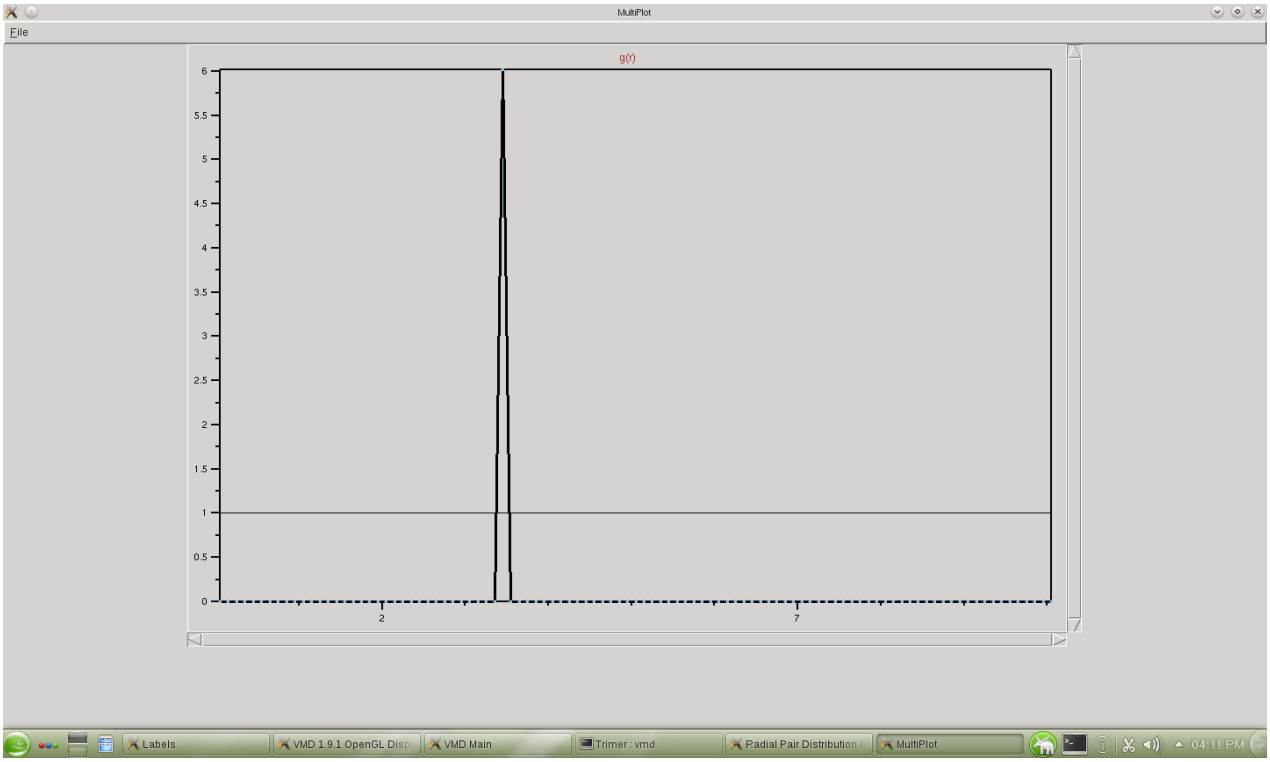
Radial Dist “O-O” Dimer –



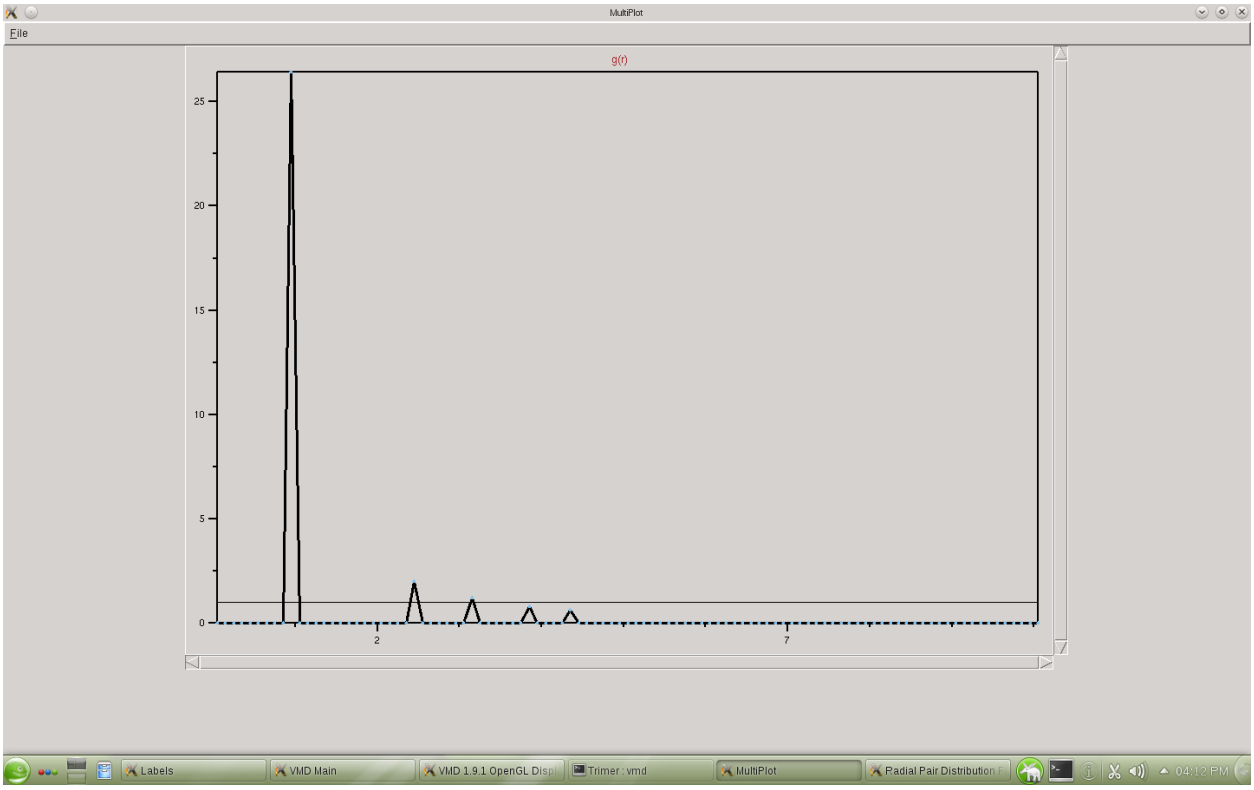
Radial Dist “O-H” Dimer –



Radial Dist “O-O” Trimer –



Radial Dist “O-H” Trimer –



Min distance and angle for Dimer –

Distance btw O-O = 3.43

Angle Between H-O-O = 17.52

Min distance and angle for Trimer –

Distance btw O-O = 3.44

Angle Between H-O-O = 6.69

Comparison –

Water Density –

Density of water is coming out to be nearly 1.07 which is pretty close to density of water at 300k “.9976”. Which have less than 10% of error, so we can tell that our force field is good enough to mimic properties of water.

With Paper –

TABLE II. Optimized geometry and dimerization energy for the linear water dimer.

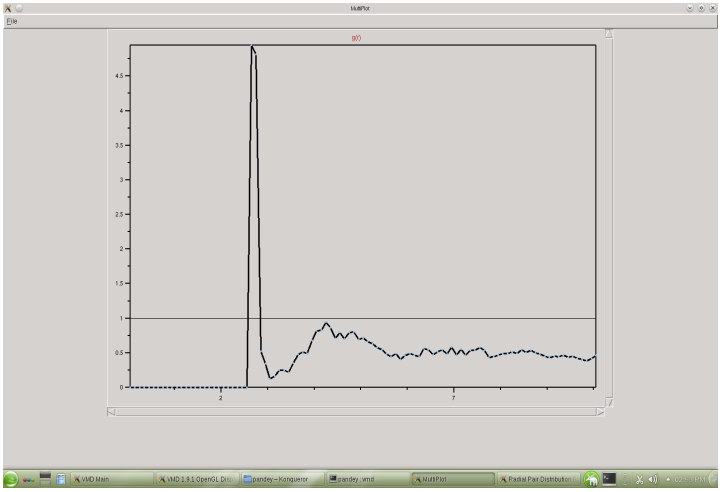
Potential	r(OO), Å	θ, deg	$-\Delta E$, kcal/mol
SPC	2.75	26	6.59
TIP3P	2.74	27	6.50
BF	2.72	47	6.06
ST2	2.85	52	6.84
TIPS2	2.79	46	6.20
TIP4P	2.75	46	6.24

In my case

R = 3.43 and Theta = 17.52 degree

Where, R is 25.1 % more than paper value and angle is 35.1% less than the paper value.

Fig – 2



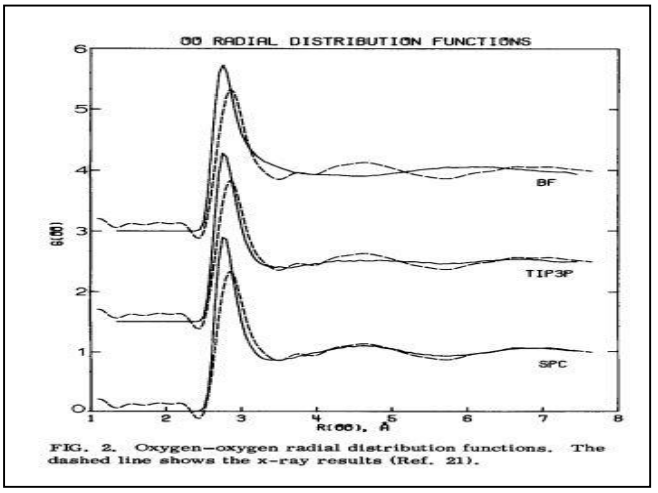
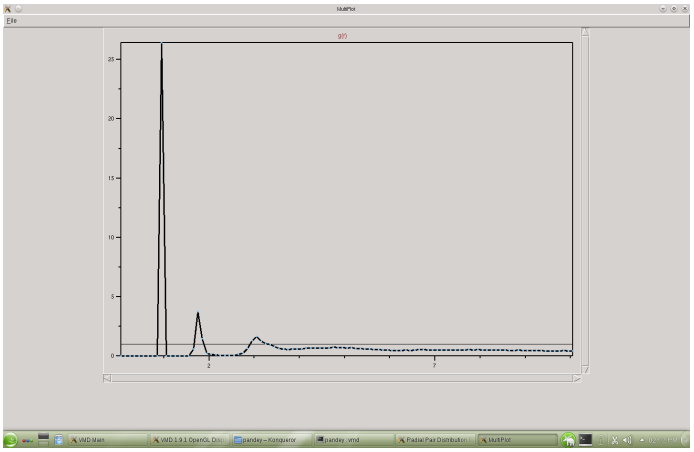


FIG. 2. Oxygen–oxygen radial distribution functions. The dashed line shows the x-ray results (Ref. 21).

Fig 5



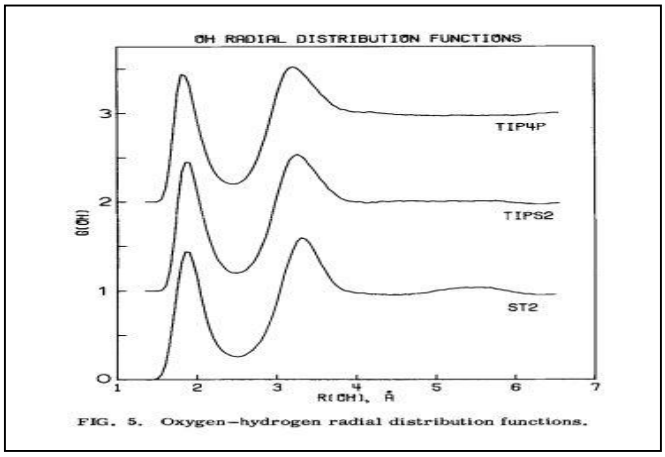


FIG. 5. Oxygen–hydrogen radial distribution functions.

We can see that It's able to mimic no. of peaks and radial position of peaks but after a threshold distance it gives too low value than the paper.