### **Meeting 1 – 25/07/2023**

* Trying to understand carbonate at high T and high P
* Interesting because this can be used for CO2 sequestration
* In the 60s X-Ray diffraction was used, nowadays you can use diamond anvil cells to carry out experiments at high P.
* It is interesting that CO2 does not seem to behave as two spheres, but instead networky things are going on
* I am going to look at sodium carbonate as a function of pressure
* Going to carry out a series of MD simulations at various pressures (Richard something model?)
* Compare structures, work out pair distribution functions
* Mark will send me some code and a pdf explaining how it works
* Fortran is a compiled language so generates executable
* Three types of ion so each pair has its own parameters
* Harmonic potential terms which covers potentials within molecules
* The smaller the cell the bigger the pressure
* Fortran is a compiled language so generates an executable
* Born Mayer potential

**Meeting 2 – 31/07/2023**

* Put in starting coordinates in the .crds file
* The three lines at the bottom are the cell lengths in atomic units
* These have been obtained from a short NPT simulation
* NVT simulations are easier to handle
* 64 molecules in cell: type 1 O, type 2 C, type 3 Na
* Simulation runs for 100 000 steps, outputting coordinates at every 100 steps (writing into poscart.out)
* Use these to produce pair distribution functions
* When doing the analysis using the rdf files, the different files represent different pairs – the one that we are probably interested in is C-C

**Email 02/08/2023**

Things you could do:

1. Work out the pressure for each run. The file “pressure.out” contains the step and pressure. You need to work out the mean pressure and the standard deviation. You’ll then be able to plot a pressure/volume curve (equation of state).

2. Calculate the coordination numbers. These are related to the integral of the first peak.

3. Work out the mean nearest neighbour separations at each pressure.

Also, you could see if anyone in the cohort uses any clever molecular graphics packages and try to look at some of the low and high pressure configurations....

Notes:

<https://en.wikibooks.org/wiki/Molecular_Simulation/Radial_Distribution_Functions>

Na2CO3

64 molecules

Na 128

C 64

O 192

Chandler p. 198: nearest neighbours comprise the first coordination shell

hdhdhd

Questions to ask Mark:

* For C-C it is hard to pick a minimum
* CNs seem inaccurate – am I doing something wrong

To discuss with Mark:

* Show the P vs V plot

Pair CN (mean) CN (median)

O-O 1.9996952206195937 1.9999718975489171

O-C 0.9999682632658408 0.9999753320851734

O-Na 4.528020040783537 4.71911613307404

C-C 3.249996059127373 3.327330468962196

C-Na 10.382161636433844 10.591981588440923

Na-Na 7.7090462833122935 7.8451359792763

C-C P5

Meeting 11/08/2023

Don’t average over pairs for separation and don’t average over pressure for CNs

Start writing!!

Noise is fine because it’s amorphous

Encountered issue: P2 is lower than P1

Might not be an issue because VdW does the same?