### **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