Homework 13 Advanced Thermodynamics
Due Wednesday November 23, 2021

LAMMPS is a molecular dynamics package that can be used for coarse grain simulation of spheres. There is a nice webpage that takes you through implementation of LAMMPS on your computer which requires some downloads and compilation. This is marginally easy to do.
https://www2.ph.ed.ac.uk/~cbrackle/lammps_tutorial.html
The first five of these simulations are doable, the sixth is challenging. I'd like you to try to do the first five simulations on your computer after downloading the package. This should give you a good idea of what is possible using LAMMPS for soft materials. This webpage was put together by Chris Brackley at Edinburgh University. He published a paper in *Nature* last year that you will find familiar once you complete the fifth example simulation. Brackley C, Gilbert N, Michieletto D, Papantonis A, Pereira MCF, Cook PR, Marenduzzo D *Complex small-world regulatory networks emerge from the 3D organisation of the human genome* Nat. Comm. **12** 5756 (2021).

For this homework, please turn in a screen shots of the final structures in each of the simulations using Ovito (a shareware package you can download, open the "dump" files in Ovito).

If you need help you can contact me or you can contact Ugochuckwu Okoli who is my graduate student and who is working more closely with LAMMPS. okoliuo@mail.uc.edu

Question:
Explain what is the "free-energy landscape" for the type of assembly mentioned in Buckley's paper and how LAMMPS allows you to explore this free-energy landscape.