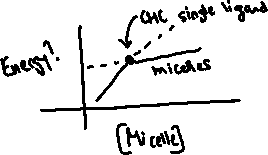
**Nanoparticle Aggregation Simulation Talk**

1. When NP’s aggregate, they lose value (how do we prevent this?)
   1. NP aggregating can cause these species to lose their nanoparticle behaviour if they cluster up close enough to become a large specie
   2. Prevention: understanding under what thermodynamic and electrostatic conditions species aggregate, will allow us to avoid those conditions when dealing with nanoparticles
2. You need to coat NP’s with a bulky, charge, soapy capping agent. The charge will minimize aggregation. Like charges repel.
3. Must simulate both NP’s and the fluid they are suspended in
4. How to simulate:
   1. LJ Potential to simulate interactions of all entities to make a molecular dynamics simulation
      1. Done – MD simulation of many instance of 1 type of entity
      2. Add multiple types of entities (to simulate capping agents and their ion competitors)
   2. Monte Carlo simulation of chemical reactions between
      1. All spheres of one type (metals)
      2. Sphere of metal with ionic species
5. CMC = critical micelle concentration. Suspension of NP’s in soapy fluid is a highly nonideal fluid



**Abstract**

* Simulate the aggregation of non-ionic capped nanoparticles that causes the minimization of Gibbs Free Energy in the system
* Apply Lennard-Jones Potential, Molecular Dynamics and Monte Carlo simulations
* MD: Approximates electro-kinetic, ultrasonic and gravitational behaviour
* MC: Simulate probability of reaction between particles

**Literature Review**

* Non-random Two Liquid (NRTL) used to develop model
  + Models fluids/surfactant only
  + System with no charge
  + Polymeric and Electrolytic system with charge distributions
  + System dealing with all sorts of components
  + Conflict: Prevent CMC aggregation when NP’s are considered
* Forms of Aggregation: Nucleation caused by the attraction of surfactants to the charges on NP
  + Growth by Diffusion
  + Aggregation
  + Autocatalytic growth: caused by low energy barrier to segregation of particles from clusters and aggregation of non-ideal atoms such as halides
* CMC Figure
  + Determine optimal surfactant concentration that causes the formation of micelles
  + Prevent clustering of surfactant around NP’s

**Algorithm**

* Start particles in perfect crystal structure
* Initialize velocity and acceleration using random number generator
* Run simulation from t = 0 to t = max time, increasing by a small time step
  + Generate new position of particles
    - Apply boundary conditions: if particle leaves the simulation box, another one enters with the same velocity, acceleration and physical properties
  + Predict new velocity using gear factor
    - Scale velocity to ensure conservation of momentum and energy in the system
  + Compute nearest neighbours
    - Compute distance between each pair of particles in the system
  + Compute Lennard Jones Potential and Force between each pair
  + Equilibration
    - If particles are close enough to bond, let them bond
    - If particles are close enough to aggregate, let them aggregate
  + Print new positions on a grid

**Results**

* Initial position of particles in the system
* Current aggregation over time shows particles wanting to aggregate (no MC simulation of reactions done, only MD on motion)
* LJ Potential figure between two particles for point after bond radius to infinity (attractive region)