# Introduction

For 8 weeks, between May 2017 and July 2017, I worked with Dr. James Brenner from the Florida Institute of Technology Chemical engineering department in Melbourne, Florida. This summer project is a part of my Independent Study course in regards to graduating with a Nanotechnology/Nanoscience minor in spring 2018.

I worked with Dr Brenner on a project to simulate the molecular dynamics of nanoparticles in solution, a project he had already started with Ayo Adebisi and James Williams.

# Objectives/Method

Using a MatLab code found in “The Working Person’s Guide to Molecular Dynamics Simulations” by Dr. David Keffer as a basis, we improve and adapt it to apply to nanoparticles as well. The original code can be found in the “MD-working\_material.pdf” file in the folder containing this report as well as the actual version of the code.

In addition to that, a class was to be created to contain the properties of most atoms in an attempt to combine that with the code to reach the goal. The original atoms class was given to me by Ayo Adebisi and can be found in the folder as well as the version with my modifications.

# Observations/Results

Most of the modifications that have been made to the code have been explained with comments. The code uses the Lennard-Jones equation for the long range energy correction and use the Gear 5 algorithm for the energy fluctuations. Modifications have been added to display the positions of the atoms at every 100 time steps.

Regarding the atoms class, many properties were added to the original file that just had atom’s name and proton number.

A couple of tests have been ran using the molviewer built-in MatLab function but nothing has been really conclusive so far

# Next Step

The next step is to find a way to incorporate the Atoms class in the code to make marker size a function of the atom number, then display using the molviewer function. Also to take in consideration: aggregation, repulsive forces, display colour.

The atoms class file is not complete yet but so far it contains up to 57 of the 95 atoms included in the excel file (noble gases not included)