Question 1

(a) The plots are "compareU.png".

Comments on the comparison: As the atomic number increases, the equilibrium distance (the distance with the minimal potential energy) increases and the absolute of the minimal potential energy increases.

(b) The plots are "He.png", "Ne.png", "Kr.png".

Question 2

The repulsive part of the LJ potential reflects the impossibility for electrons with the same spin to occupy the same region of space. If we don't consider the repulsive part, the potential energy will drop faster and faster when r becomes closer and closer to zero. Ultimately, the potential energy is negative infinity when $r=0$, and all the atoms occupy the same region of space, which is obviously unphysical.

Question 3

Using different data spanning time periods, I got different results of He density.

data spanning	1 ps	2ps	5ps	10ps	20ps	100ps
He density (g/ml)	-8.020×10^{4}	3.157×10^{-3}	1.114×10^{-3}	9.441×10^{-4}	8.415×10^{-4}	8.037×10^{-4}

From the results above we can see, the calculated density is closer to the actual density which is 8.058×10^{-4} g/ml if I use longer data spanning. This validates the argodic hypothesis. When I use data spanning of 1ps, I even got a negative value. This is because the absolute value of the slope of the fitted line is the largest.

It can be found that the longer the data spanning is, the smaller the absolute value of the slope is. (The density is stable in long data spanning.)

Question 4.

The distance between atom 1 and atom 2 $r_{12}=1.1 < 1.4 \times R_{OH}$

——— atom 1 and atom 3 $r_{13}=0.922 < 1.4 \times R_{OH}$

——— atom 2 and atom 3 $r_{23}=1.273 > 1.4 \times R_{HH}$.

so atom 1 and 2 are bonded, atom 1 and 3 are bonded, atom 2 and 3 are not bonded.

so we need to consider the L-J potential for atom 2 and 3, and the bond stretch between atom 1 and 2, and the bond stretch between atom 1 and 3, and the angle bend between H-O-H.

$$E = 4\varepsilon(H)\left(\left(\frac{\sigma(H)}{r_{23}}\right)^{12}-\left(\frac{\sigma(H)}{r_{23}}\right)^{6}\right) + K_{OH}(r_{12}-R_{OH})^2 + k_{OH}(r_{13}-R_{OH})^2 +$$

$$k_{HOH}\left(\theta_{HOH} - \arctan\left(\frac{9}{2}\right)\right)^2$$

$$= 417.09 \text{ kJ/mol}$$

For a single H_2O molecule, the energy is

$$\frac{417.09 \text{ kJ/mol}}{N_A} = 6.93 \times 10^{-22} \text{ kJ}.$$