

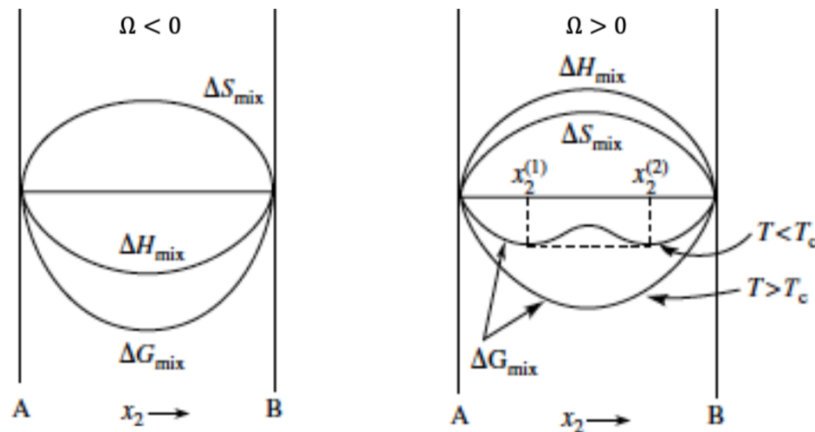
The change in the free energy in the regular solution expressed as:

$$\Delta G_{mix} = \Omega x_1 x_2 - nRT[x_1 \ln(x_1) + x_2 \ln(x_2)]$$

There are 2 cases for omega, and it influence the heat mix term.

$$\Delta H_{mix} = \Omega x_1 x_2; \Omega = \frac{z}{2}(N_1 + N_2)(2\varepsilon_{12} - \varepsilon_{11} - \varepsilon_{22})$$

For the regular solution.



Consider  $\Omega = 0.08$  there will be miscibility gap between A and B.

Algorithms to draw the Temperature concentration curve, represent the solubility limits.

In first step I draw general curve

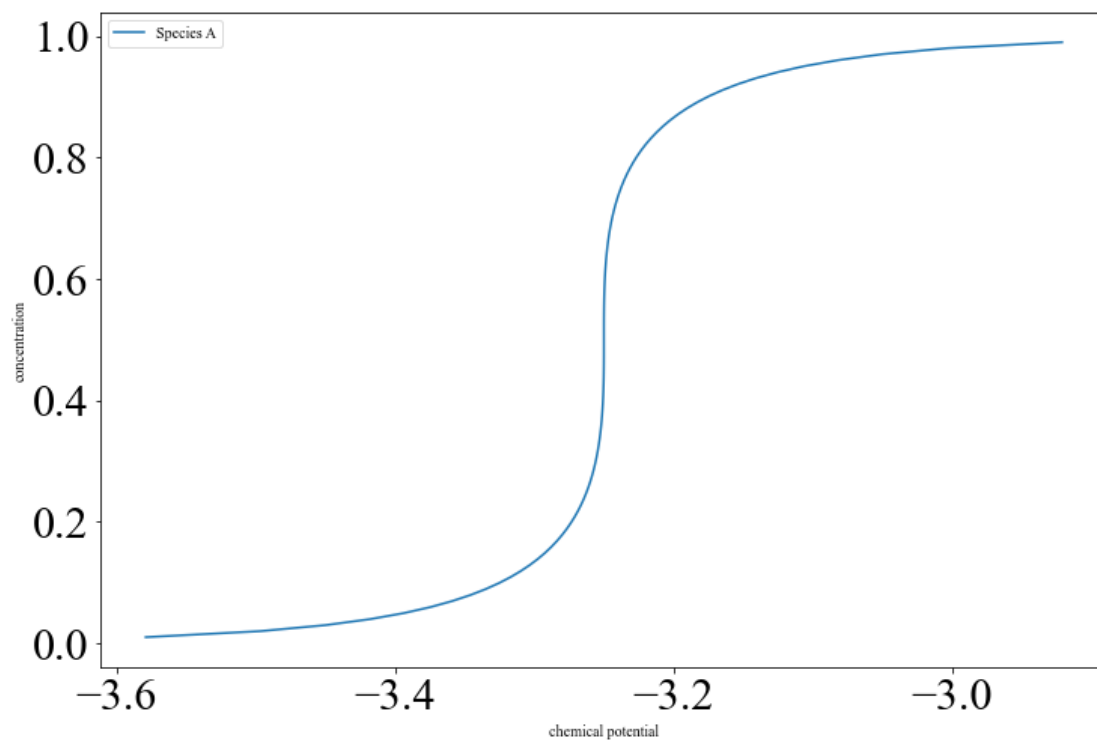
And then choose arbitrary concentration (0.1,0.2,0.3,0.4,0.5)

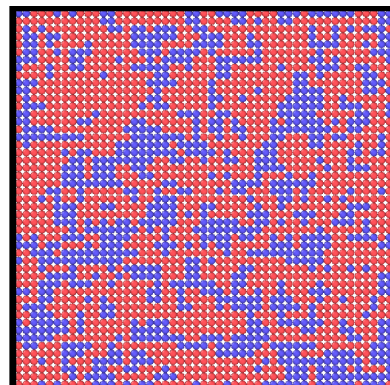
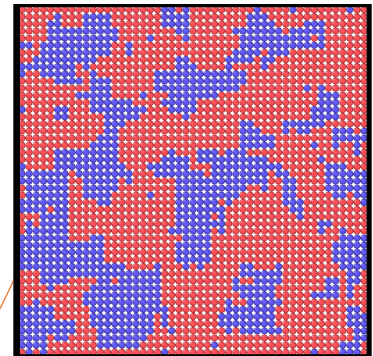
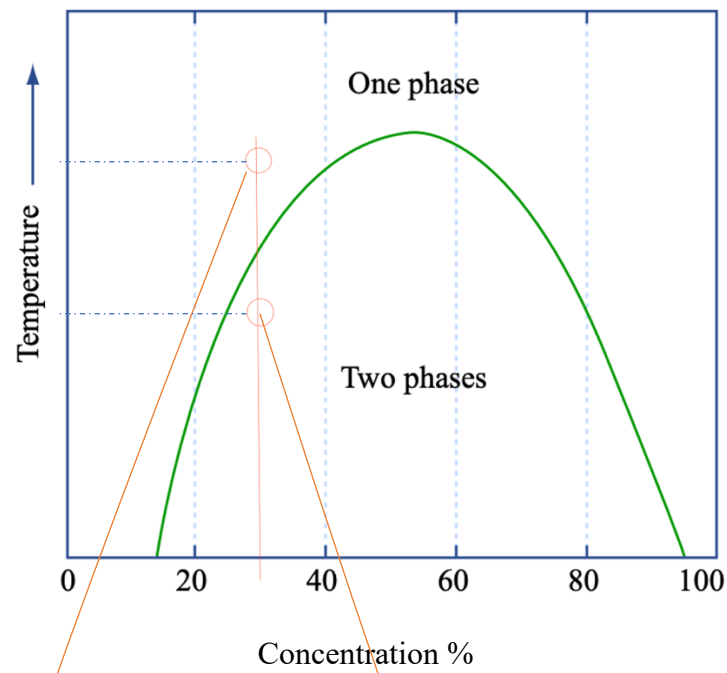
I used bisection algorithm to find the closet value based on visualization of cluster, OVito.

By using the data to plot a figure using python, showing the minimum and maximum values taken.

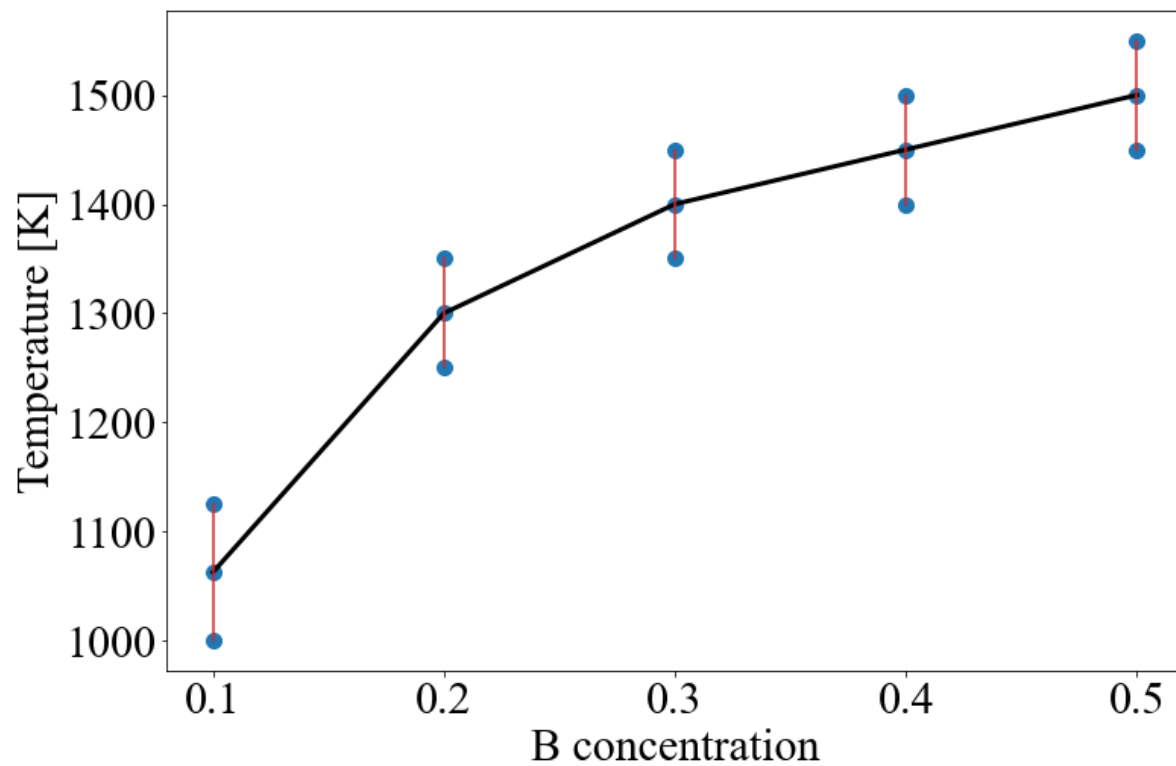
Finally, plot the figure based on the mean values.

**Plot of concentration\_chemical potential:**





**Plot of Temperature\_Concentration:**  
The final figure are as follows:



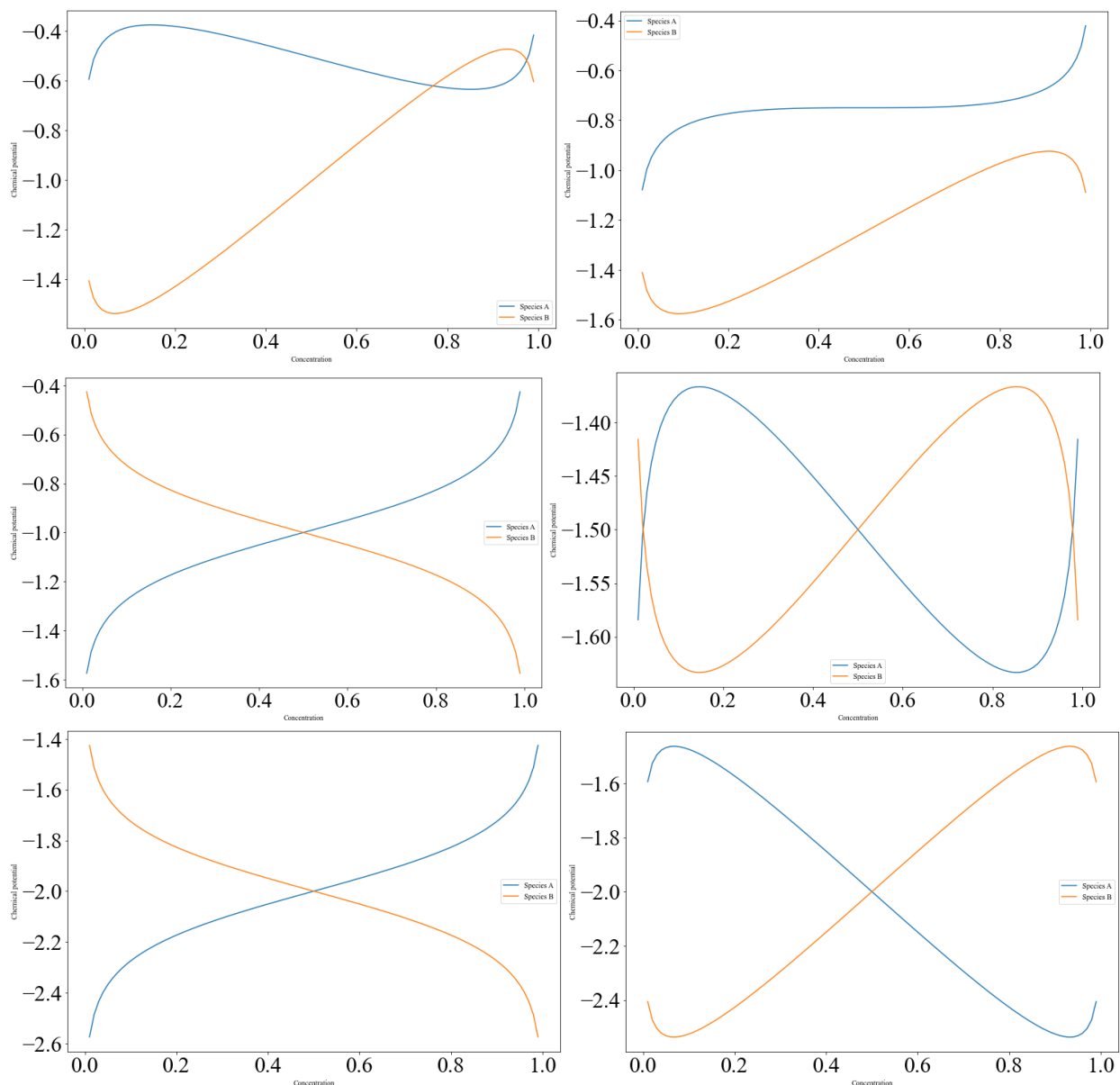
**Plot of Chemical potential\_concentration:**

changing the interaction energies  $e_{11}$ ,  $e_{22}$ , and  $e_{12}$  will affect the calculated chemical potentials, which are plotted as a function of concentration. Specifically, the chemical potential is a measure

of the free energy of a species, which depends on the interaction energy between that species and other species in the system.

Similarly, changing the magnitudes of  $e_{22}$  and  $e_{12}$  will affect the balance of forces between species B-B and A-B, respectively, and will result in changes to the chemical potentials and the shape and position of the chemical potential curves.

Therefore, changing the interaction energies between species in a system can have a significant impact on the behavior of the system and the properties of its components, including their concentrations and chemical potentials.



**Plot for concentration\_chemical potential:**

changing the values of  $e_{11}$ ,  $e_{22}$ , and  $e_{12}$  will affect the calculated chemical potentials and, consequently, the plot of the chemical potentials versus concentration.

Specifically,  $e_{11}$ ,  $e_{22}$ , and  $e_{12}$  are the interaction energies between the species A-A, B-B, and A-B, respectively. These interaction energies contribute to the chemical potential of each species, which is calculated using the formula:

$$\begin{aligned}\mu_A &= e_{11} * x_A + e_{12} * x_B + k_B * T * \log(x_A / (1 - x_A)) \\ \mu_B &= e_{22} * x_B + e_{12} * x_A + k_B * T * \log(x_B / (1 - x_B))\end{aligned}$$

where  $x_A$  and  $x_B$  are the mole fractions of species A and B, respectively.

Thus, changing the values of  $e_{11}$ ,  $e_{22}$ , and  $e_{12}$  will change the contributions of each interaction energy to the chemical potential, and consequently, the shape and position of the chemical potential curves on the plot.

For example, if you increase the magnitude of  $e_{22}$  relative to  $e_{11}$  and  $e_{12}$ , the chemical potential curve for species B will be shifted downwards and will have a steeper slope, while the chemical potential curve for species A will be shifted upwards and will have a shallower slope. This is because the increased interaction energy between B-B has made species B less favorable and species A more favorable, relative to their concentrations, resulting in the observed changes in chemical potential.

