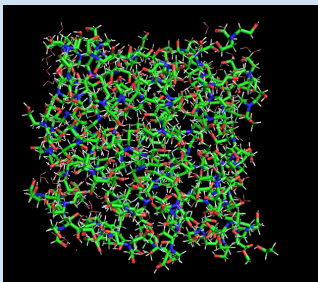
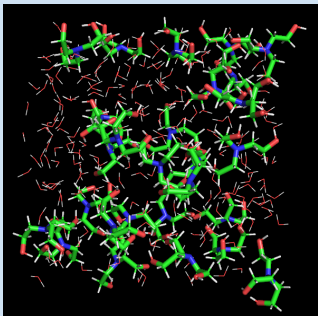
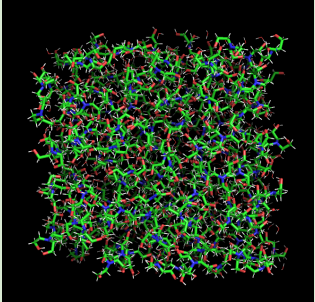
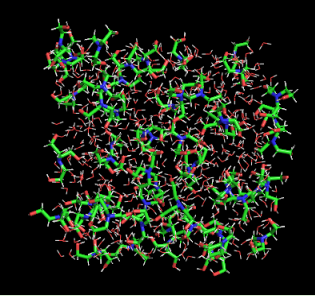
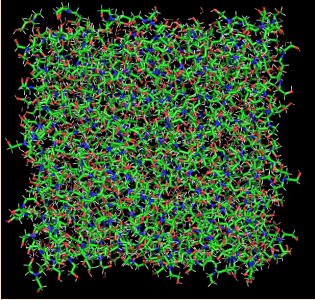
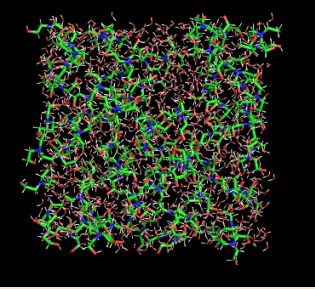


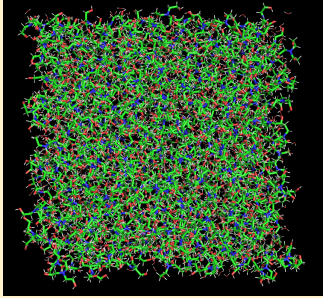
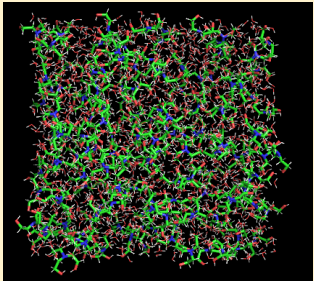
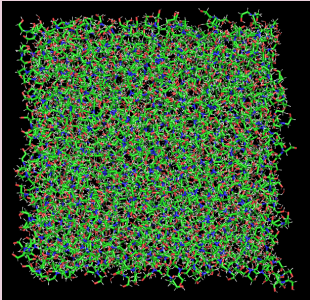
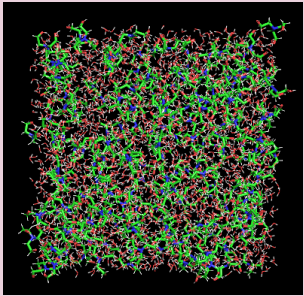
Experiments/Simulations Log

09/05/2024

- Running system size tests for Hmix and density
 - Molecule: 'OCCN(CCO)CCO'
 - Sizes: 500,1000,1500,2000
 - Finished
- Hmix+density - **Test box size**
 - Molecule: OCCN(CCO)CCO
 - Water model: TIP3P-FB
 - Experiment
 - Hmix = -1.221 kJ/mol (Mole fraction ~50/50)
 - Density = 1.0747210000000005 g/mL (Mole Fraction ~10/90)

System size	Property	Snapshot	Calculated Value	Wall time
250 (jobid = 17743315)	Hmix	 a=b=c=31.130	-1.376 +/- 0.127 kJ/mol	00:40:13
	Density	 a=b=c=22.870	1.104 +/- 0.001 g/mL	

500 (jobid = 17738172)	Hmix	 a=b=c=39.262	-0.771 +/- 0.099 kJ/mol	00:45:19
	Density	 a=b=c=28.969	1.105 +/- 0.001 g/mL	
1000 (jobid = 17738200)	Hmix	 a=b=c=49.575	-1.015 +/- 0.064 kJ/mol	01:00:53
	Density	 a=b=c=36.430	1.104 +/- 0.001 g/mL	

1500 (jobid = 17738201)	Hmix	 a=b=c=56.559	-1.897 +/- 0.060 kJ/mol	01:24:58
	Density	 a=b=c=41.673	1.105 +/- 0.000 g/mL	
2000 (jobid = 17738202)	Hmix	 a=b=c=62.281	-1.403 +/- 0.059 kJ/mol	01:50:03
	Density	 a=b=c=46.006	1.103 +/- 0.000 g/mL	