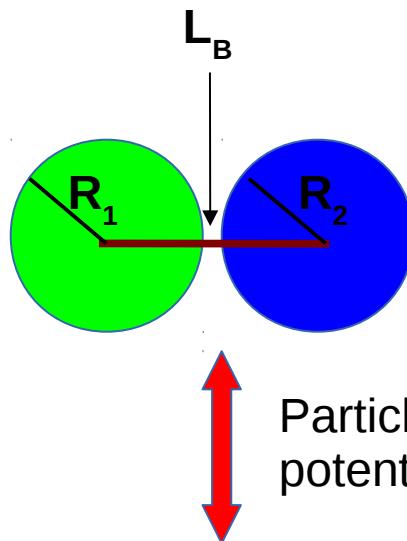


Results from Nested Sampling of 8 dimer systems at various kappa values

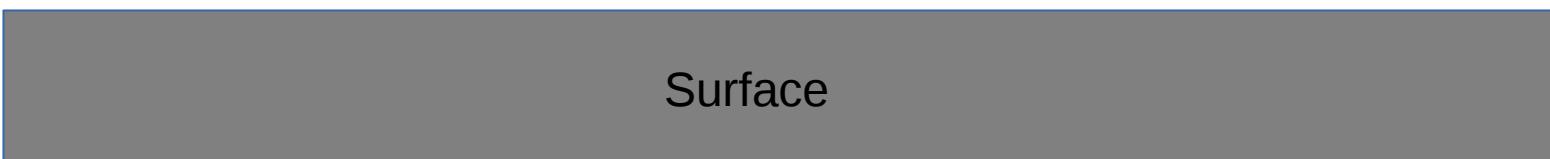
Last updated:1-31-14

Model System

One unit or dimer is composed of 2 oppositely charged particles, with radii R_1 and R_2 respectively, bound together by a rigid bond of length L_B



Particle-Particle interaction, E , given by:
$$E = E_{\text{ScreenedElectostatic}} + E_{\text{Colloid}}$$



Dimer Parameters 1

$R_1 = 1.0$

$R_2 = 2.0$

$Ae_1 = 1000.0$

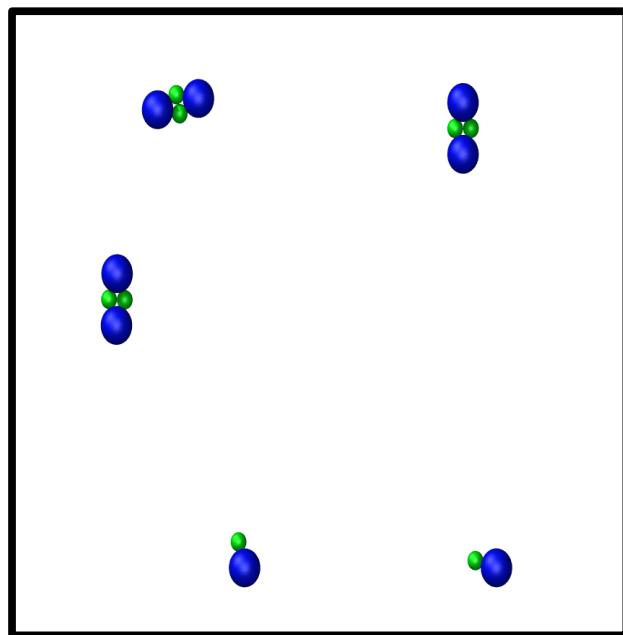
$Ae_2 = 5000.0$

$L_B = 3.0$

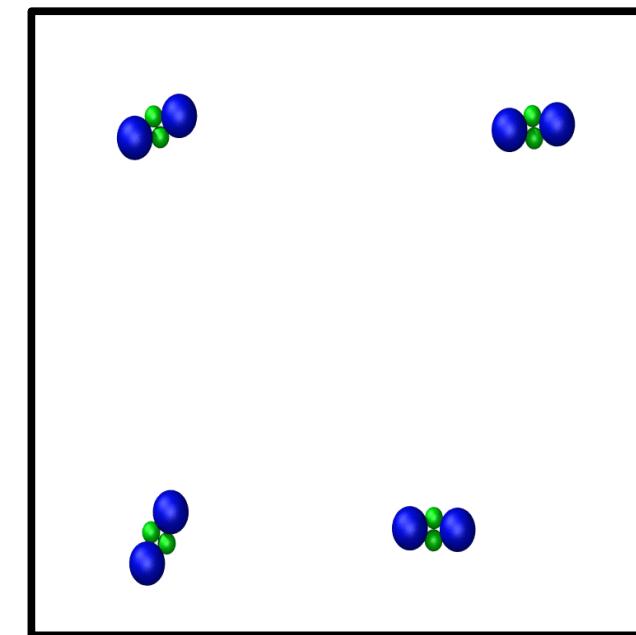
Ae values are the screened electrostatic energy-distance prefactor

Kappa 0.1

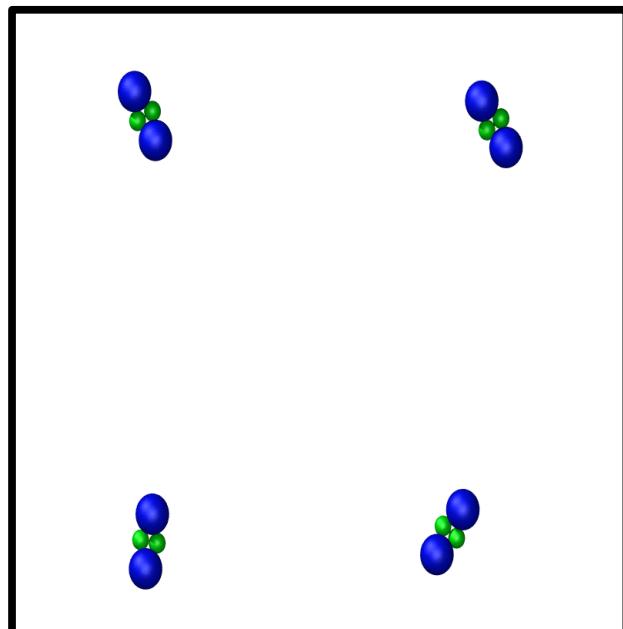
Lowest energy configuration sampled by each trial



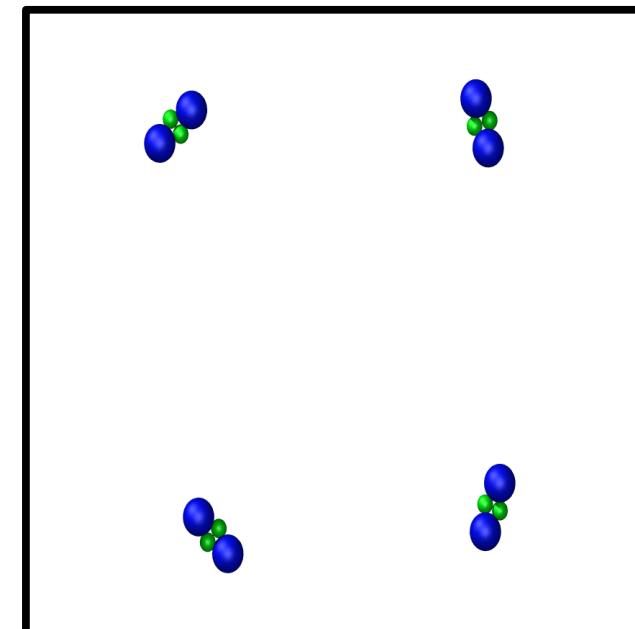
Trial1
 $E=-255.8005$



Trial2
 $E=-277.0781$



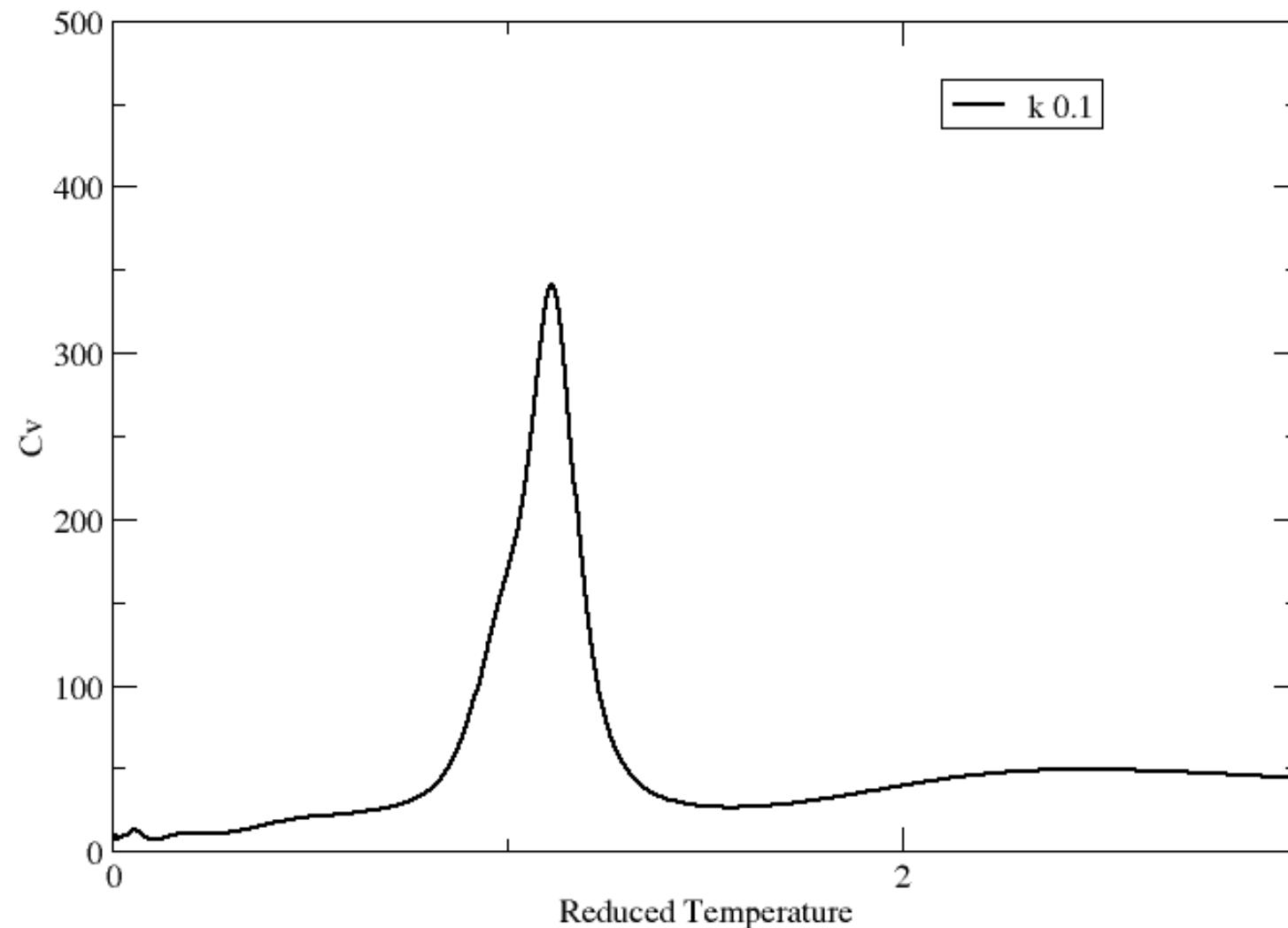
Trial3
 $E=-278.1242$



Trial4
 $E=-278.0427$

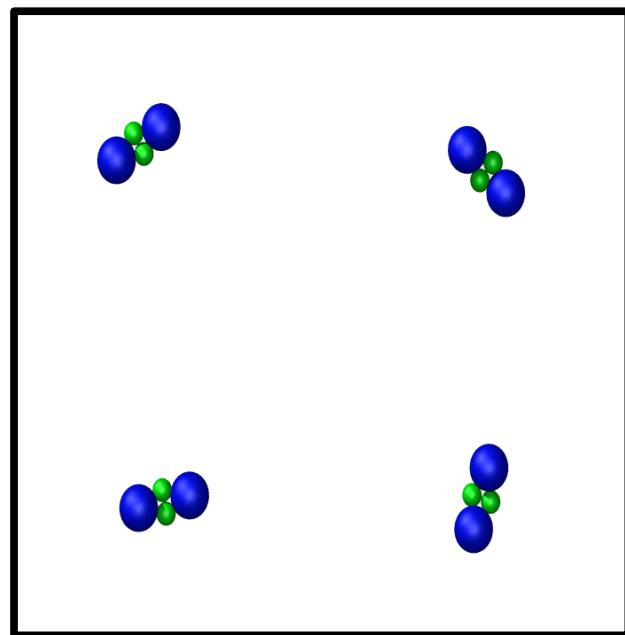
**Note squares do not reflect actual simulation box sizes

Average Heat Capacity of 4 Trials

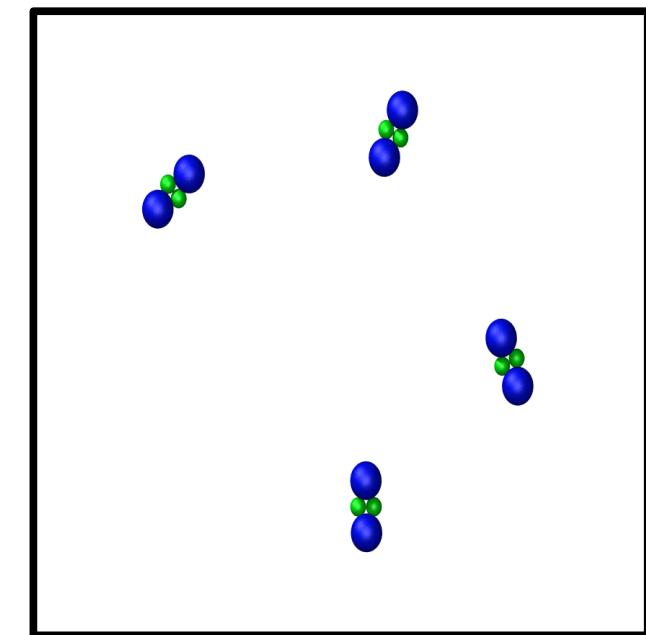


Kappa 0.2

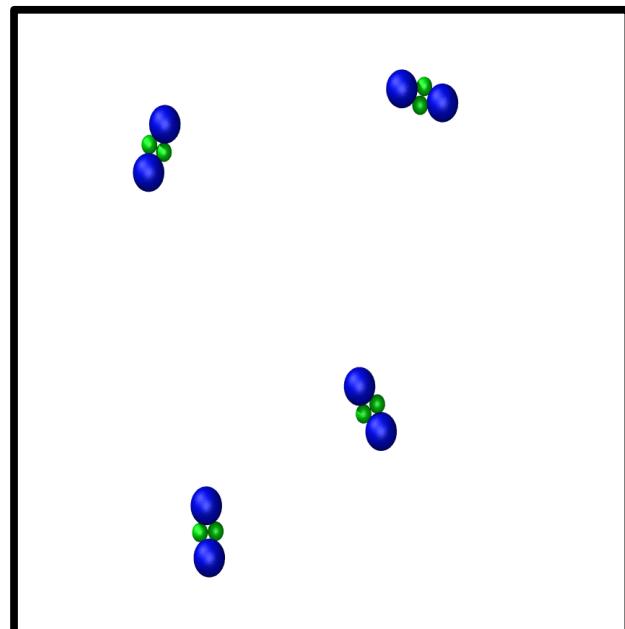
Lowest energy configuration sampled by each trial



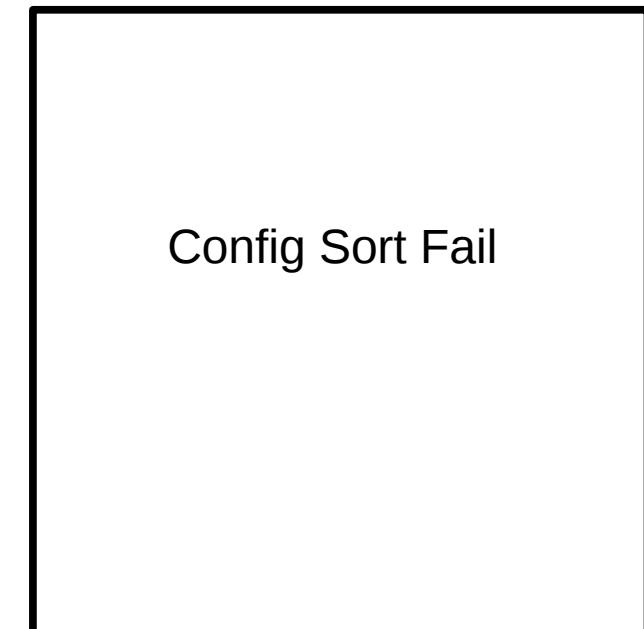
Trial1
 $E=-340.5298$



Trial2
 $E=-340.0578$

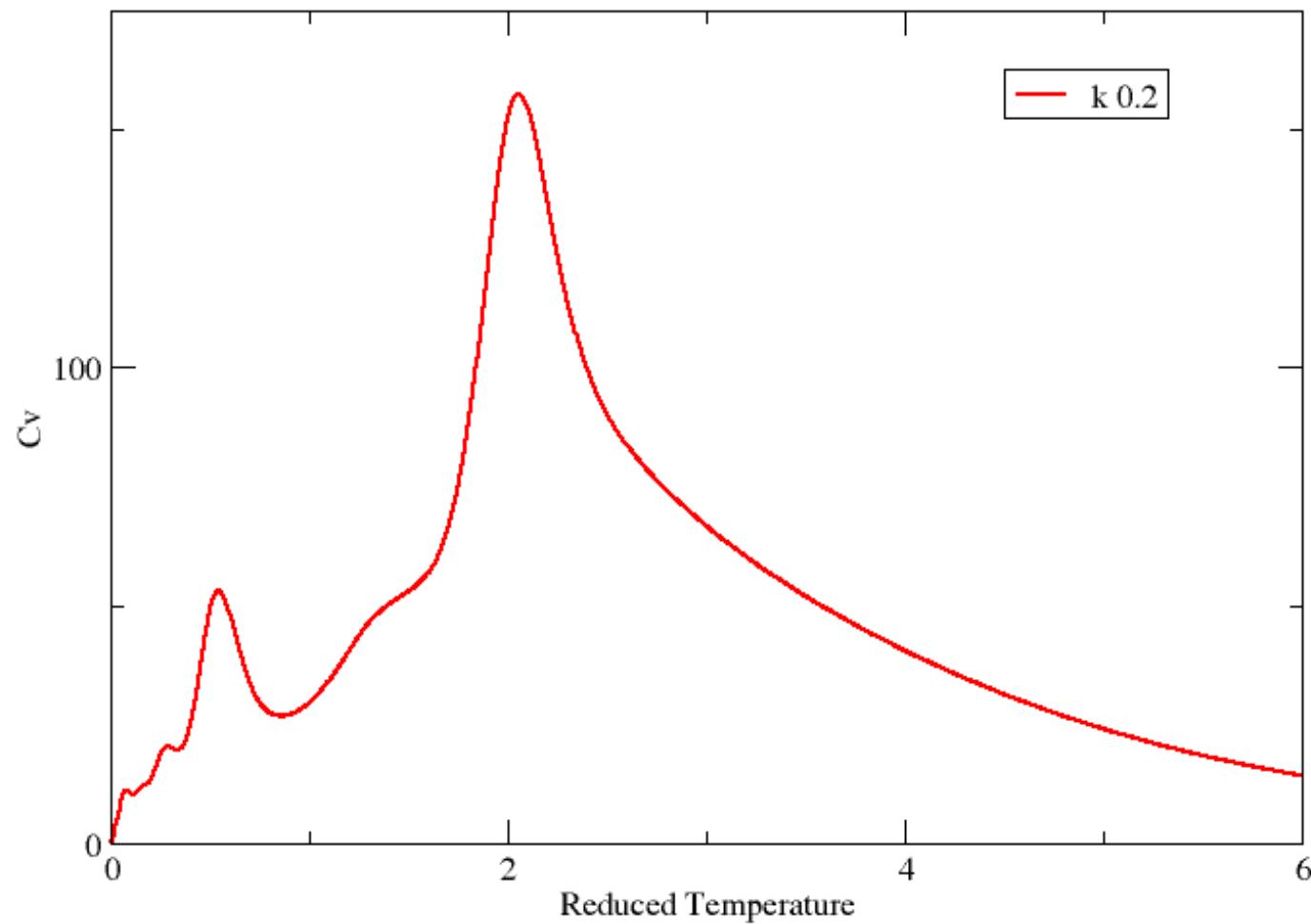


Trial3
 $E=-340.4434$



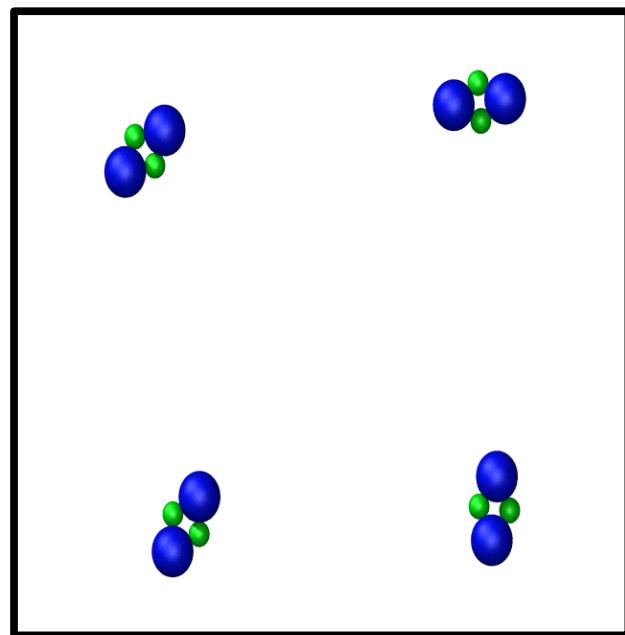
Trial4
 $E=$

Average Heat Capacity of 4 Trials

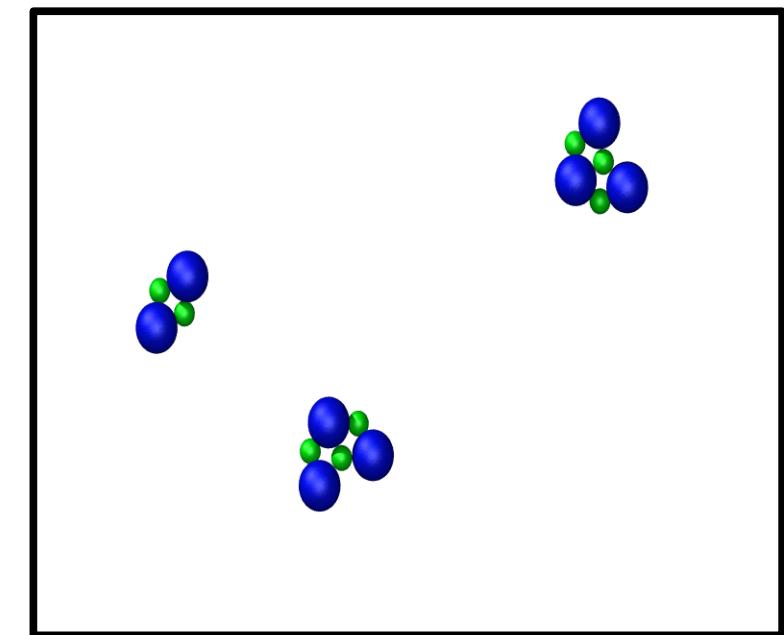


Kappa 0.3

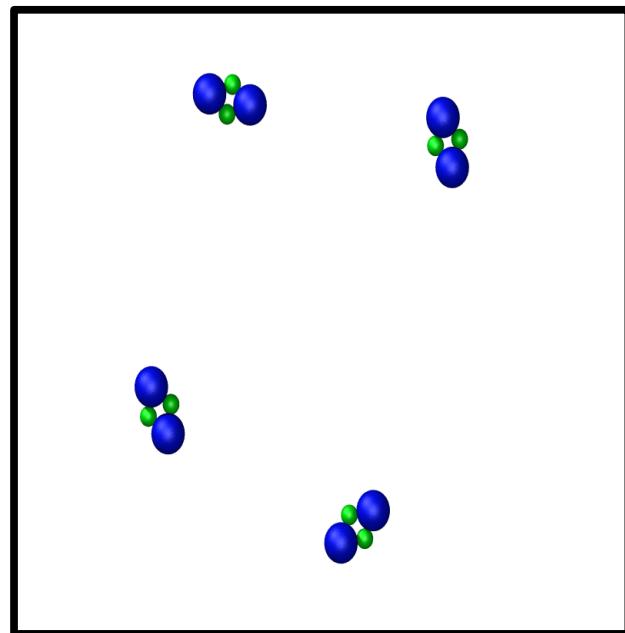
Lowest energy configuration sampled by each trial



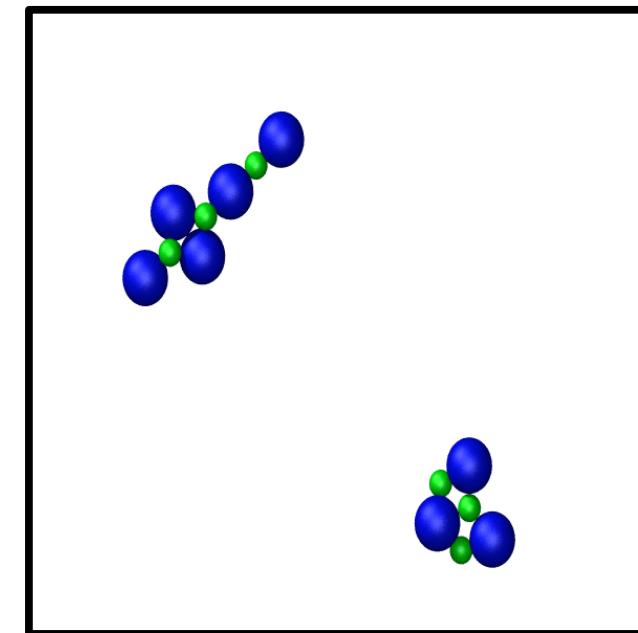
Trial1
 $E=-374.2729$



Trial2
 $E=-392.8401$

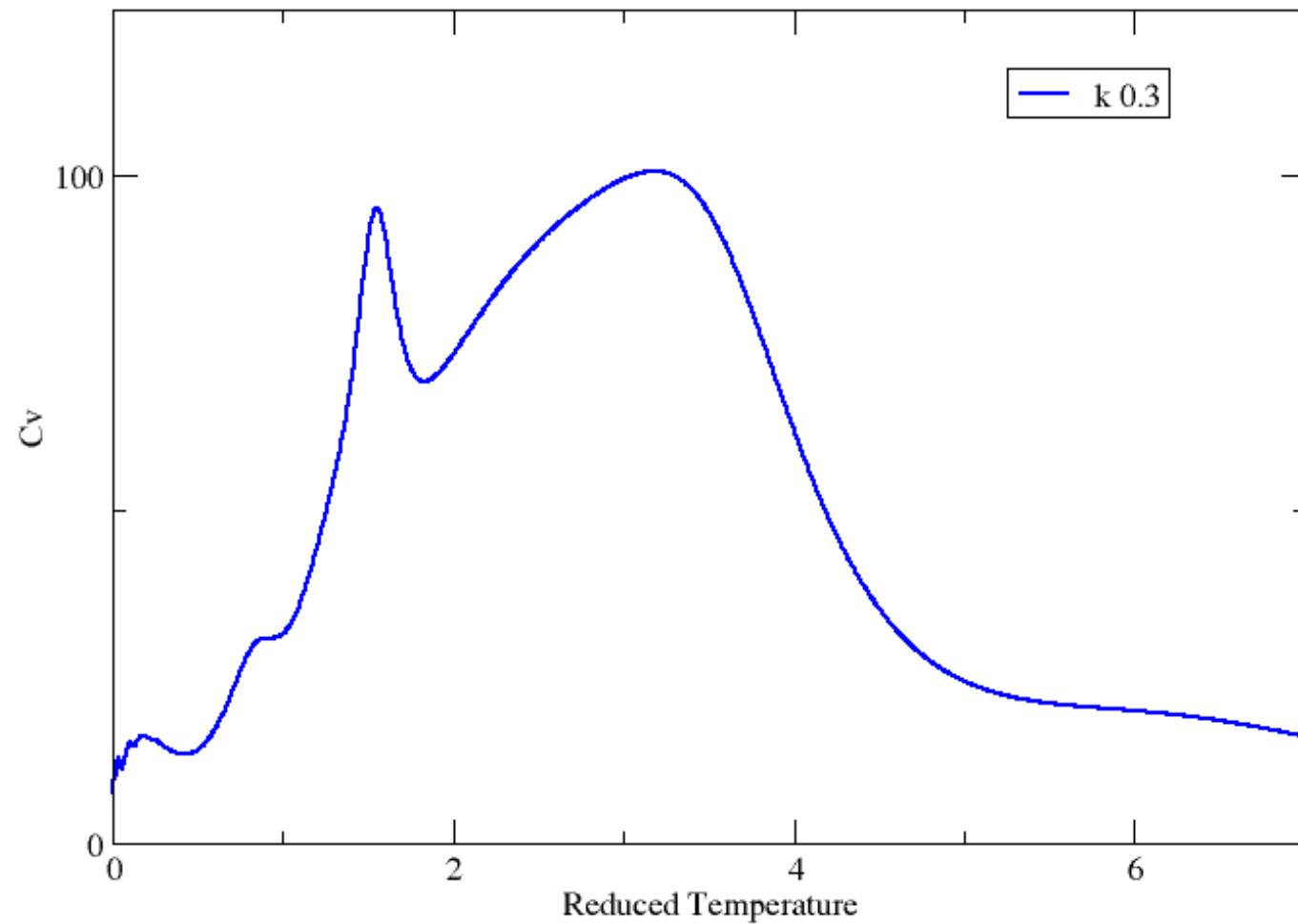


Trial3
 $E=-374.2443$



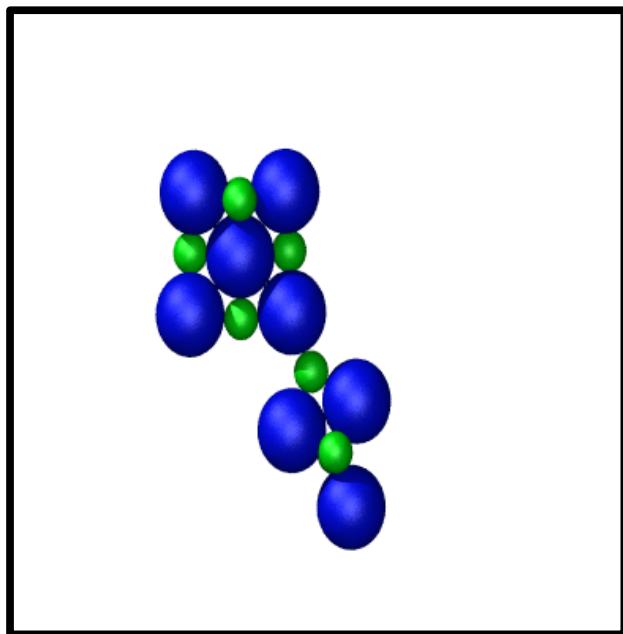
Trial4
 $E=-433.1157$

Average Heat Capacity of 4 Trials

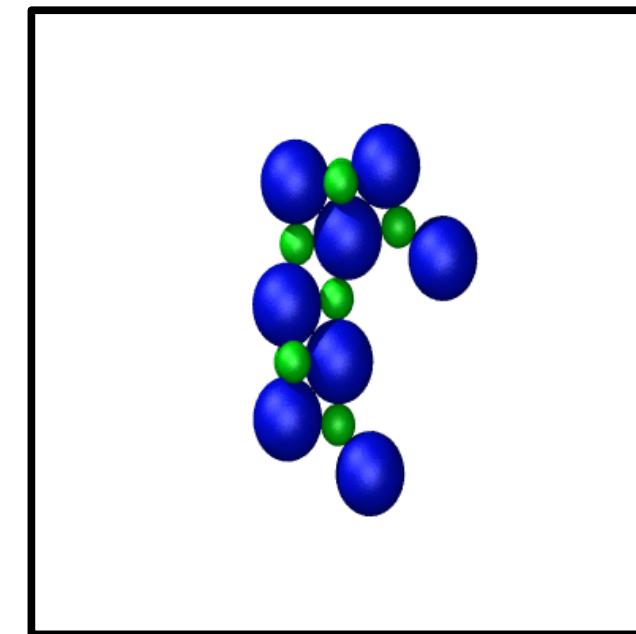


Kappa 0.4

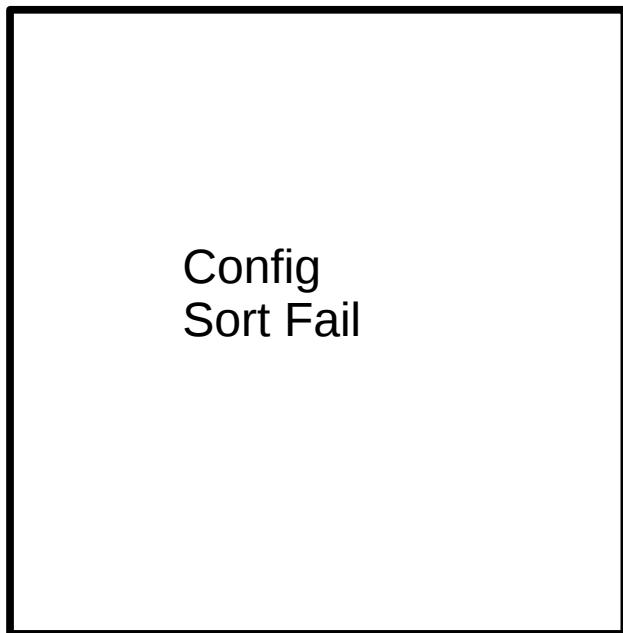
Lowest energy configuration sampled by each trial



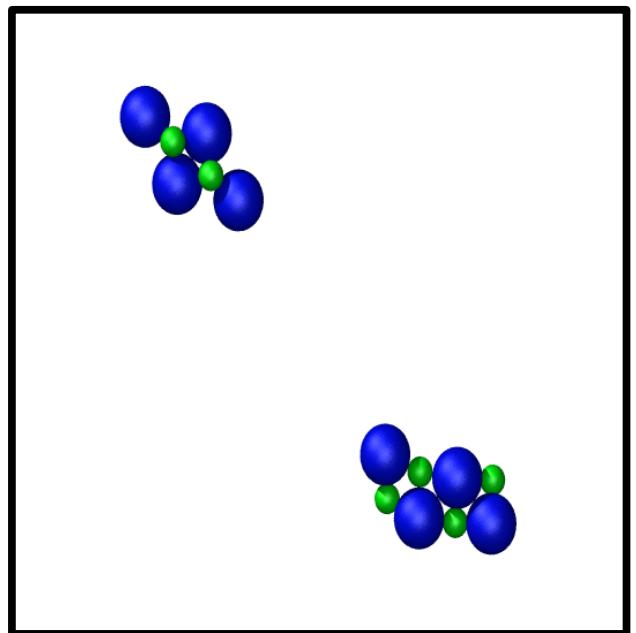
Trial1
 $E=-507.9783$



Trial2
 $E=-503.7722$

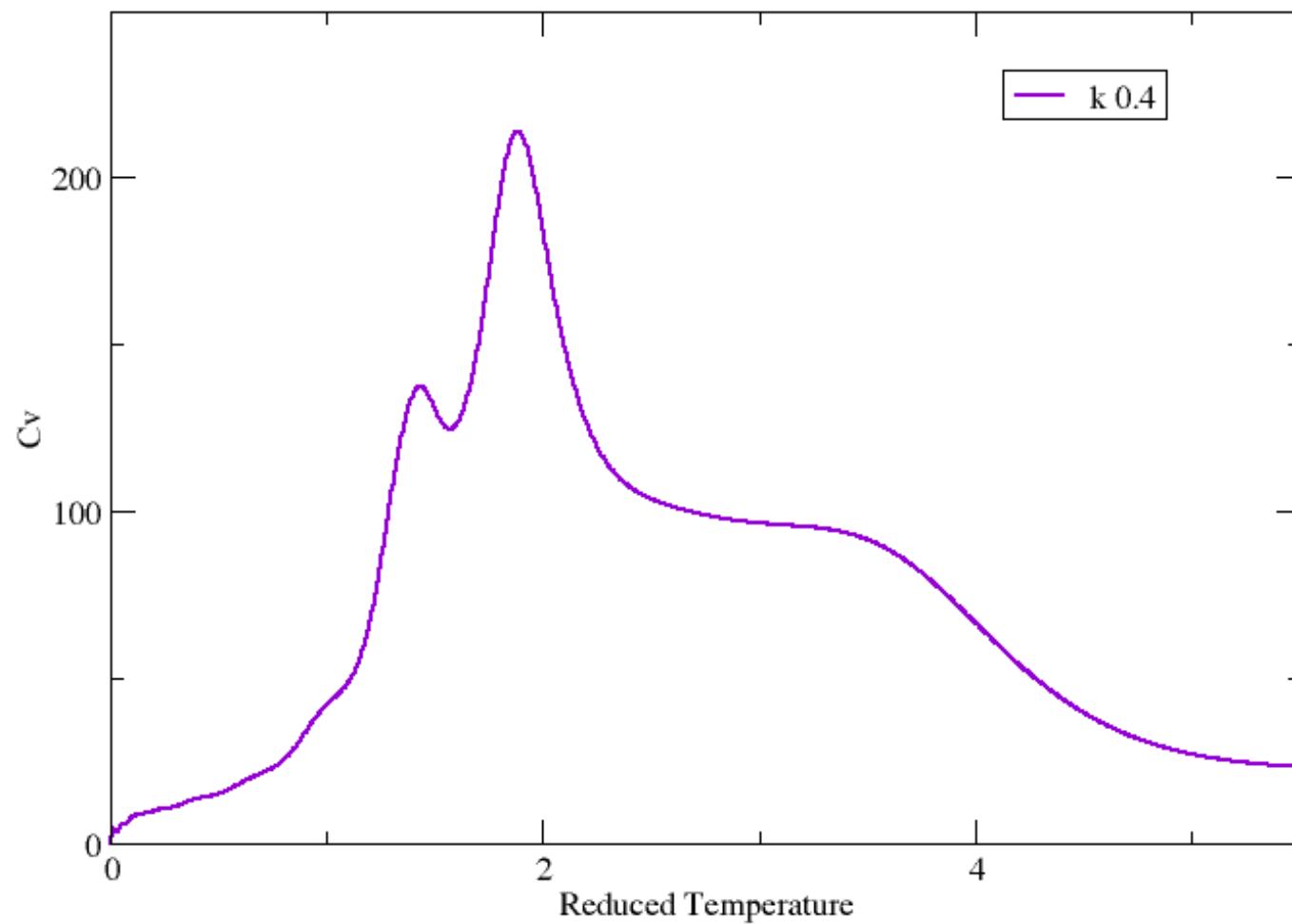


Trial3
 $E=$



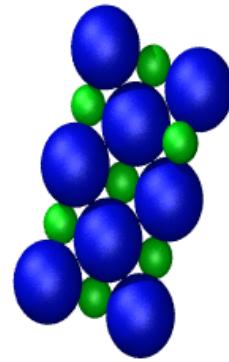
Trial4
 $E=-466.1653$

Average Heat Capacity of 4 Trials

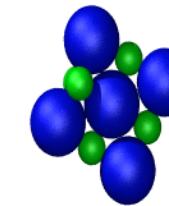


Kappa 0.5

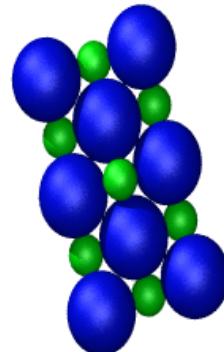
Lowest energy configuration sampled by each trial



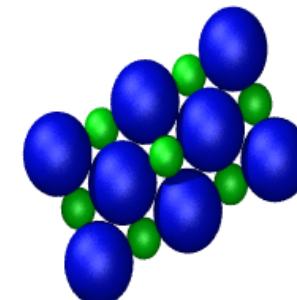
Trial1
 $E=-544.0891$



Trial2
 $E=-491.8303$

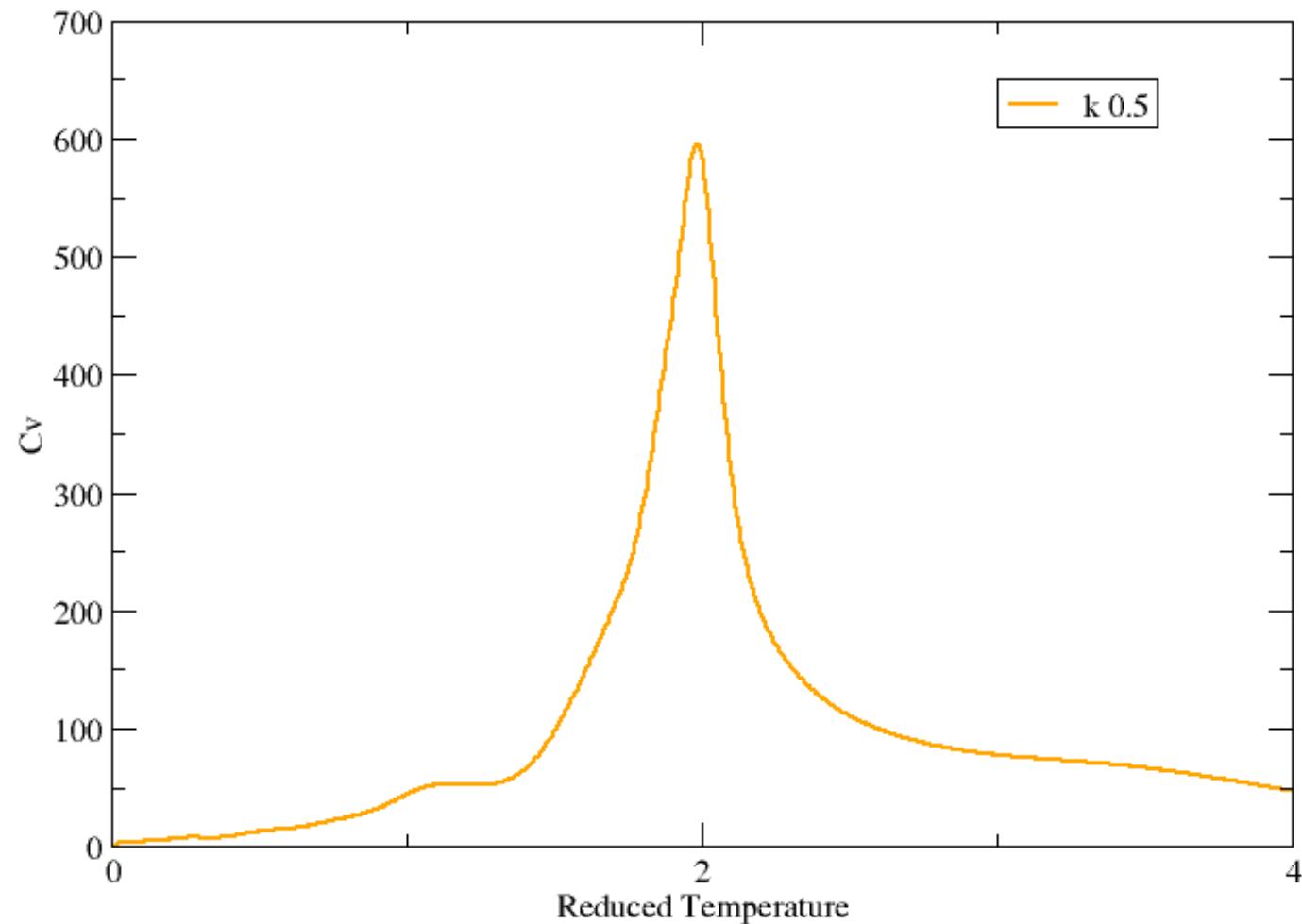


Trial3
 $E=-562.3748$



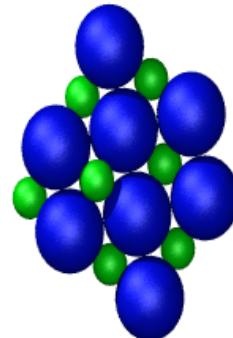
Trial4
 $E=-563.4063$

Average Heat Capacity of 4 Trials

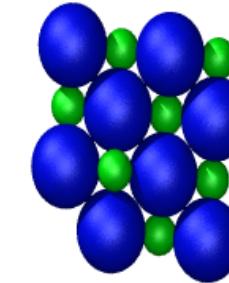


Kappa 0.6

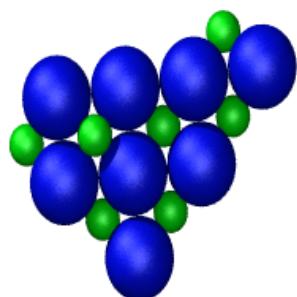
Lowest energy configuration sampled by each trial



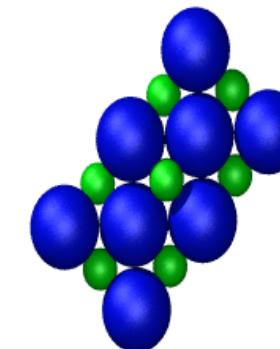
Trial1
 $E=-539.1593$



Trial2
 $E=-541.1890$

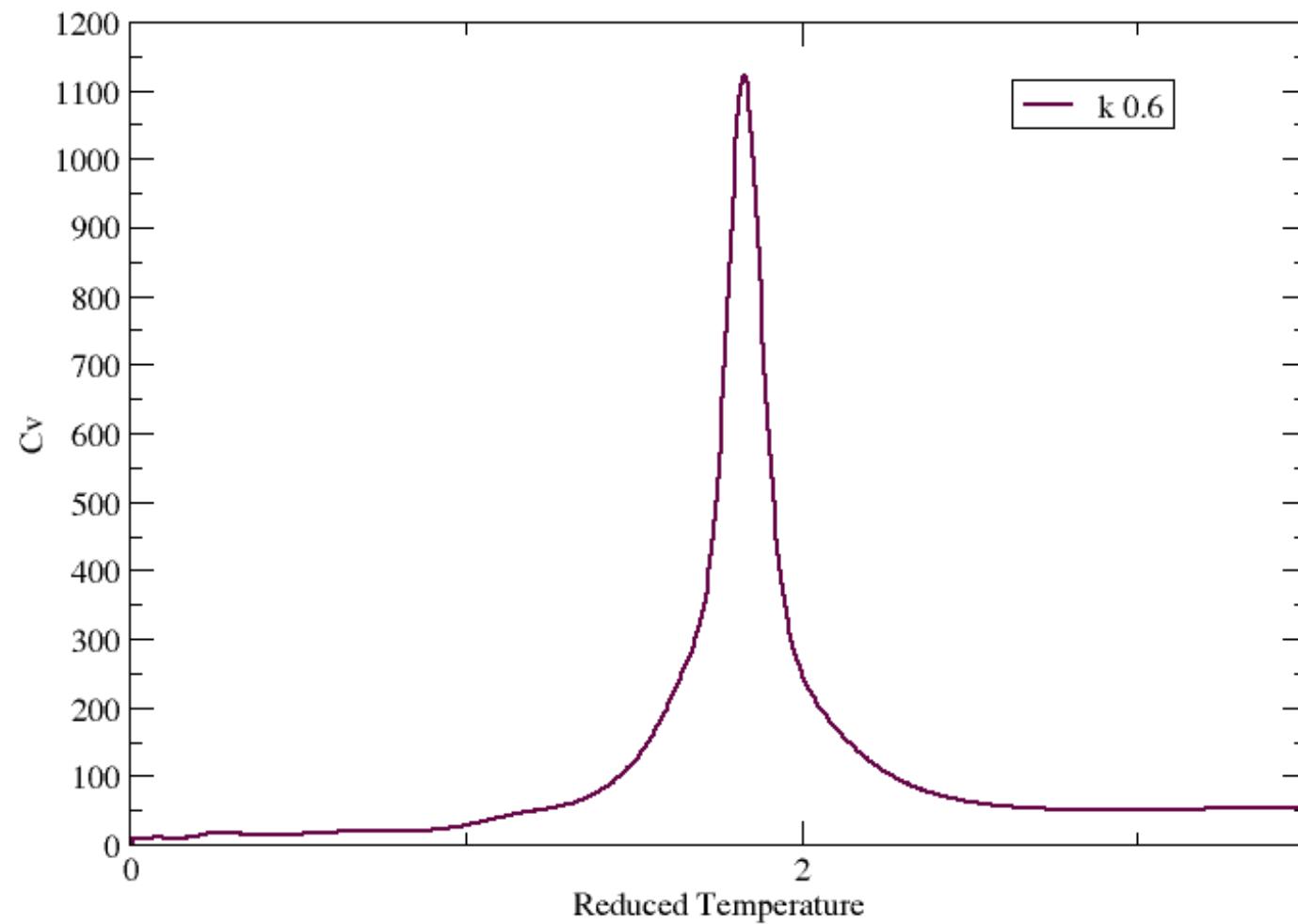


Trial3
 $E=-524.8218$



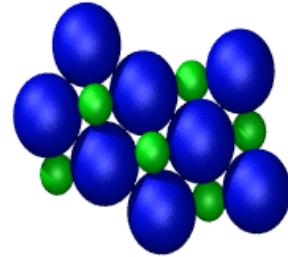
Trial4
 $E=-534.4316$

Average Heat Capacity of 4 Trials

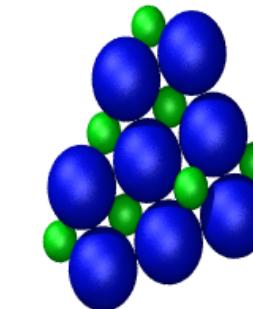


Kappa 0.7

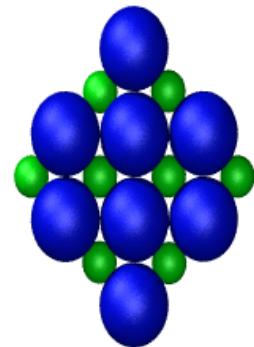
Lowest energy configuration sampled by each trial



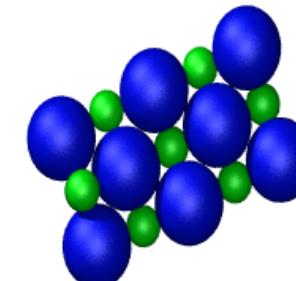
Trial1
 $E=-507.6010$



Trial2
 $E=-507.6662$

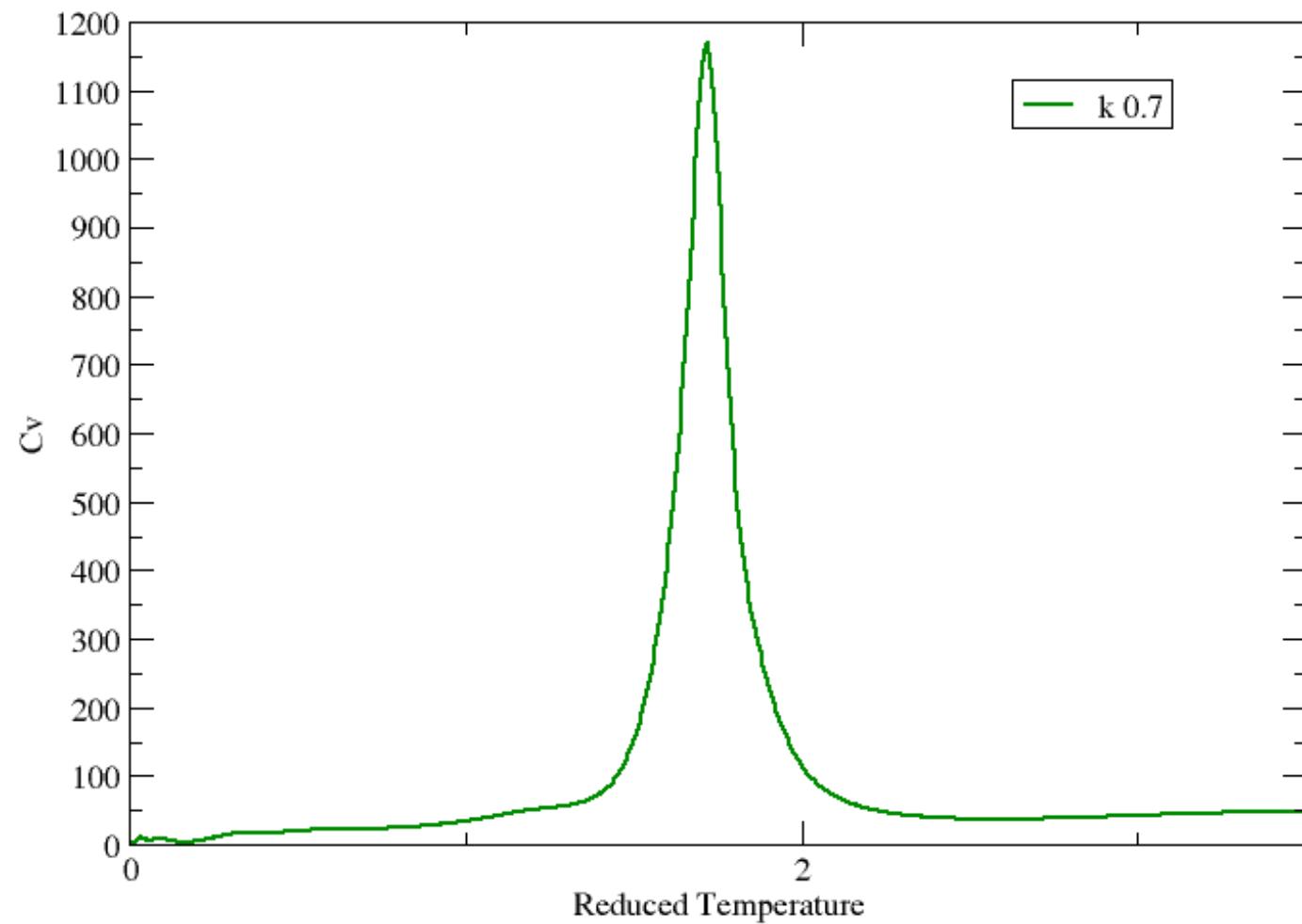


Trial3
 $E=-501.7859$



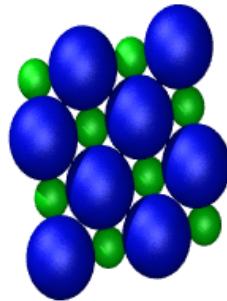
Trial4
 $E=-488.8038$

Average Heat Capacity of 4 Trials

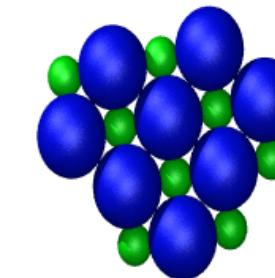


Kappa 0.8

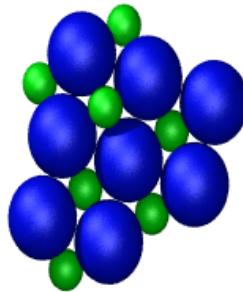
Lowest energy configuration sampled by each trial



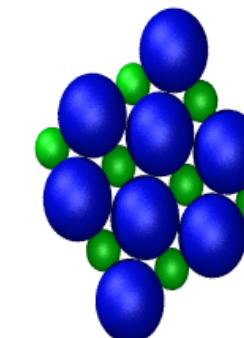
Trial1
 $E=-479.4432$



Trial2
 $E=-478.0672$

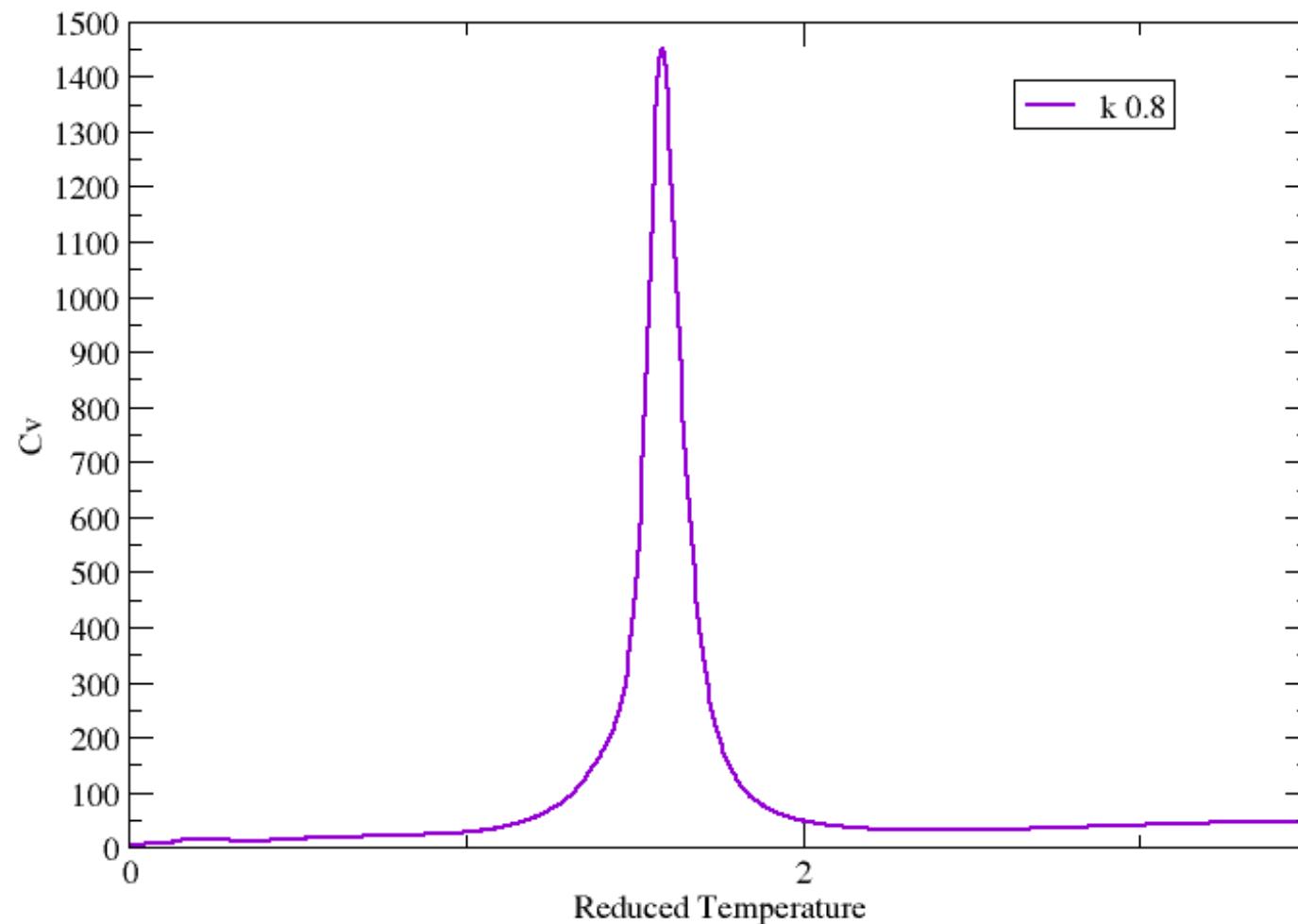


Trial3
 $E=-486.3589$



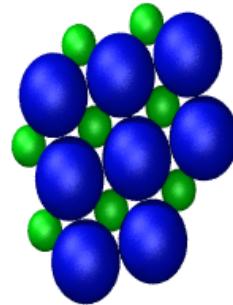
Trial4
 $E=-479.2595$

Average Heat Capacity of 4 Trials

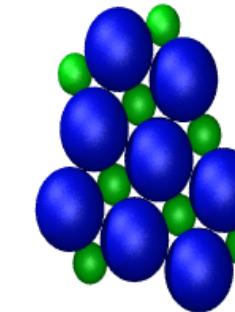


Kappa 0.9

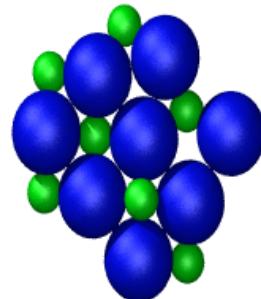
Lowest energy configuration sampled by each trial



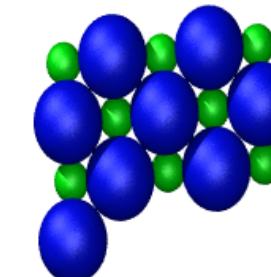
Trial1
 $E=-463.7348$



Trial2
 $E=-465.1443$

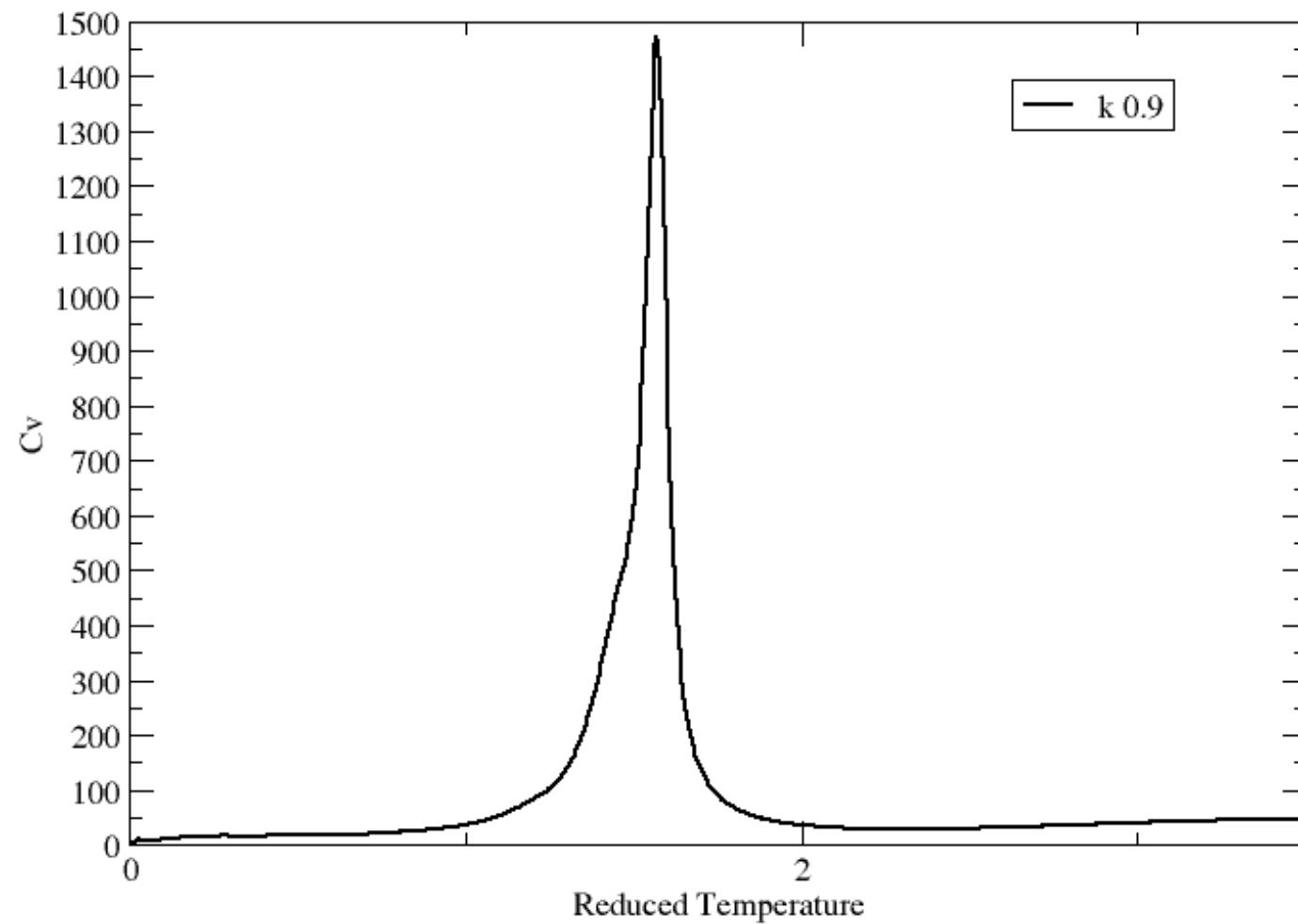


Trial3
 $E=-455.3308$



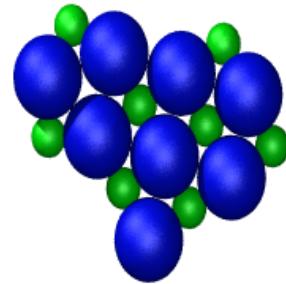
Trial4
 $E=-446.8173$

Average Heat Capacity of 4 Trials

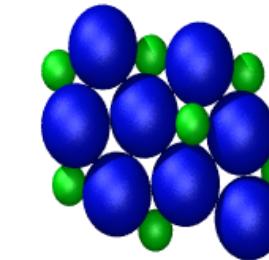


Kappa 1.0

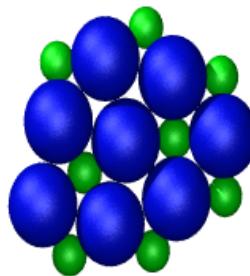
Lowest energy configuration sampled by each trial



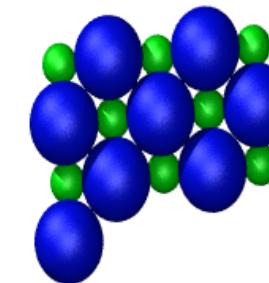
Trial1
 $E=-446.8748$



Trial2
 $E=-452.8659$

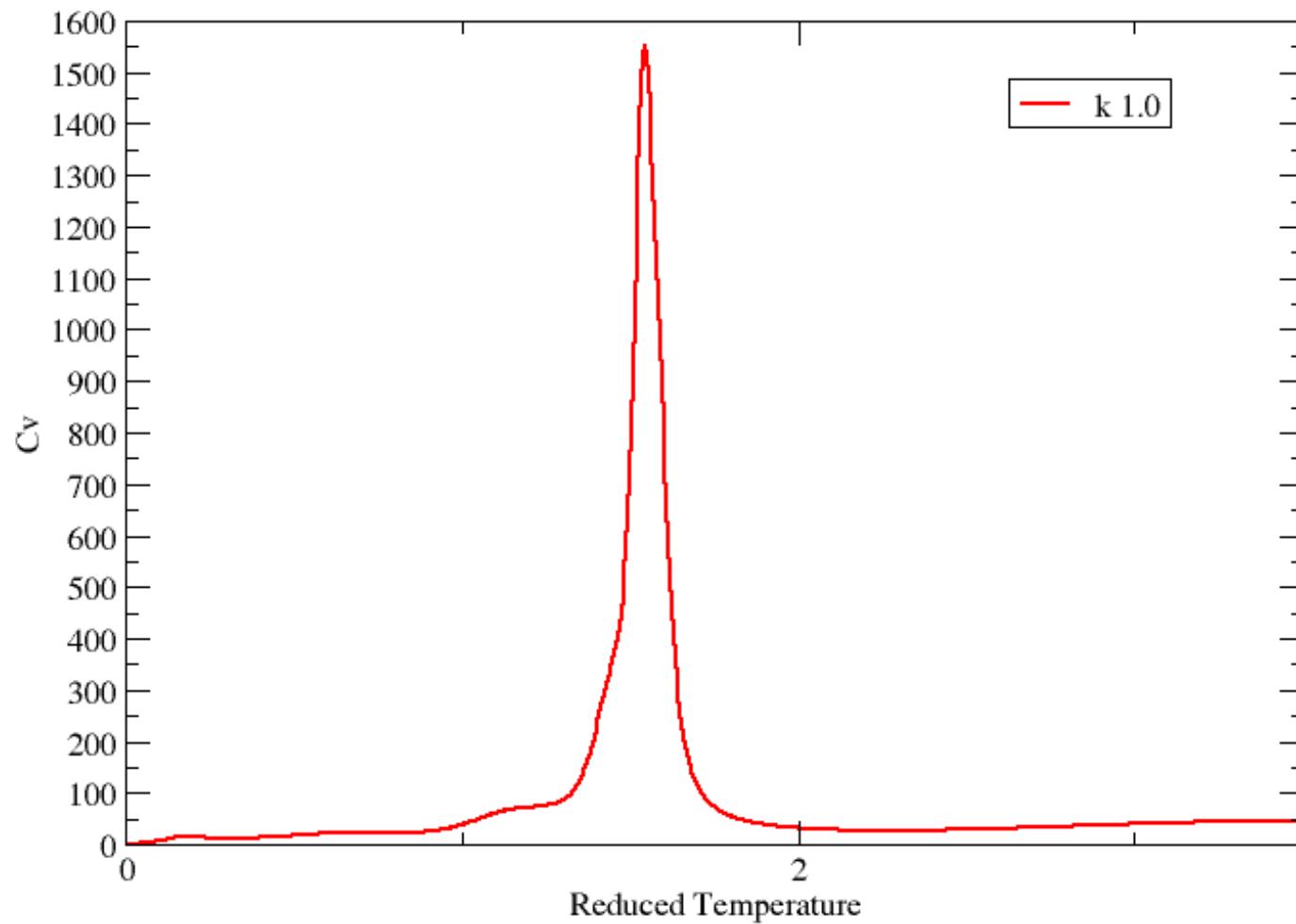


Trial3
 $E=-452.9231$

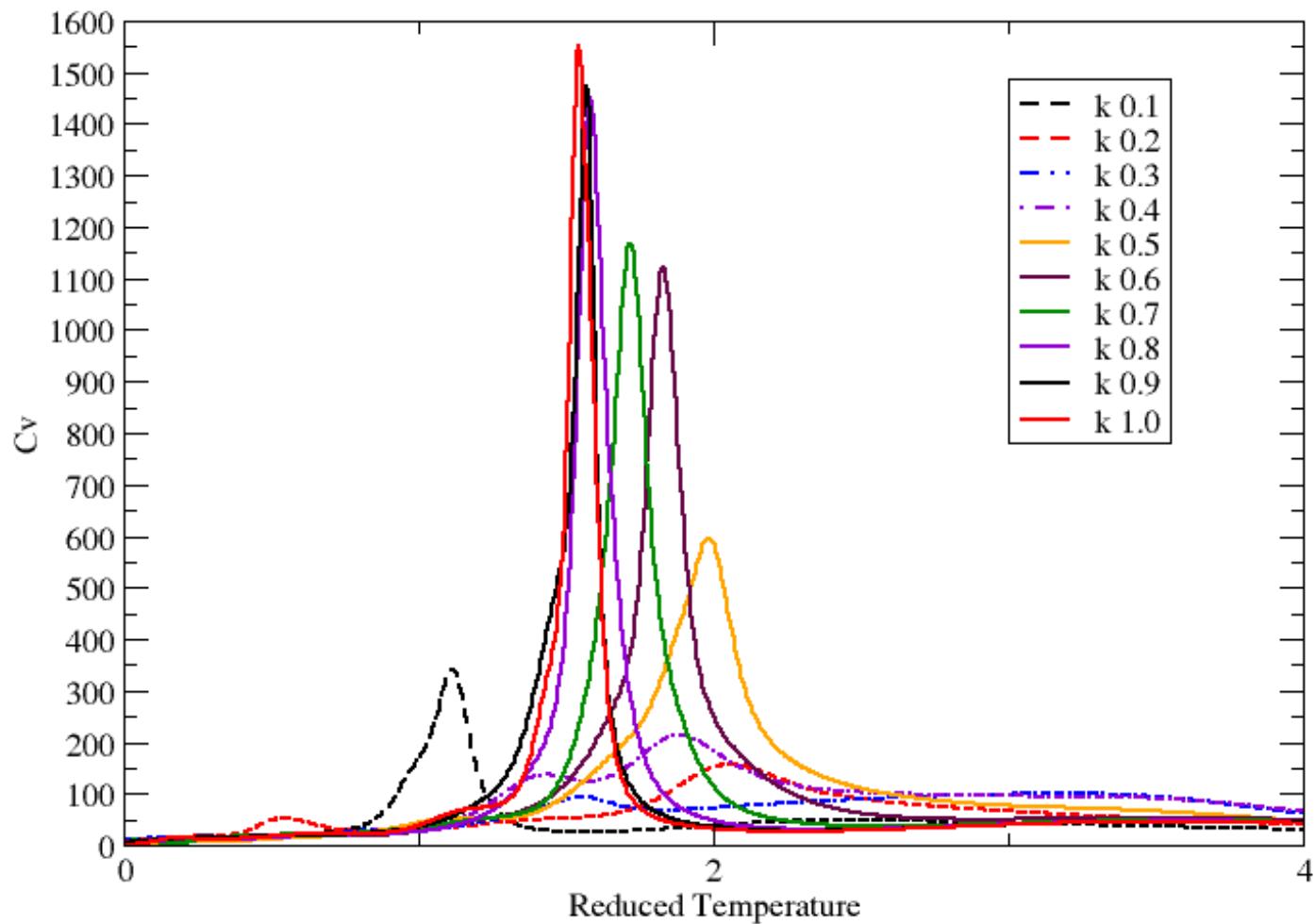


Trial4
 $E=-442.9135$

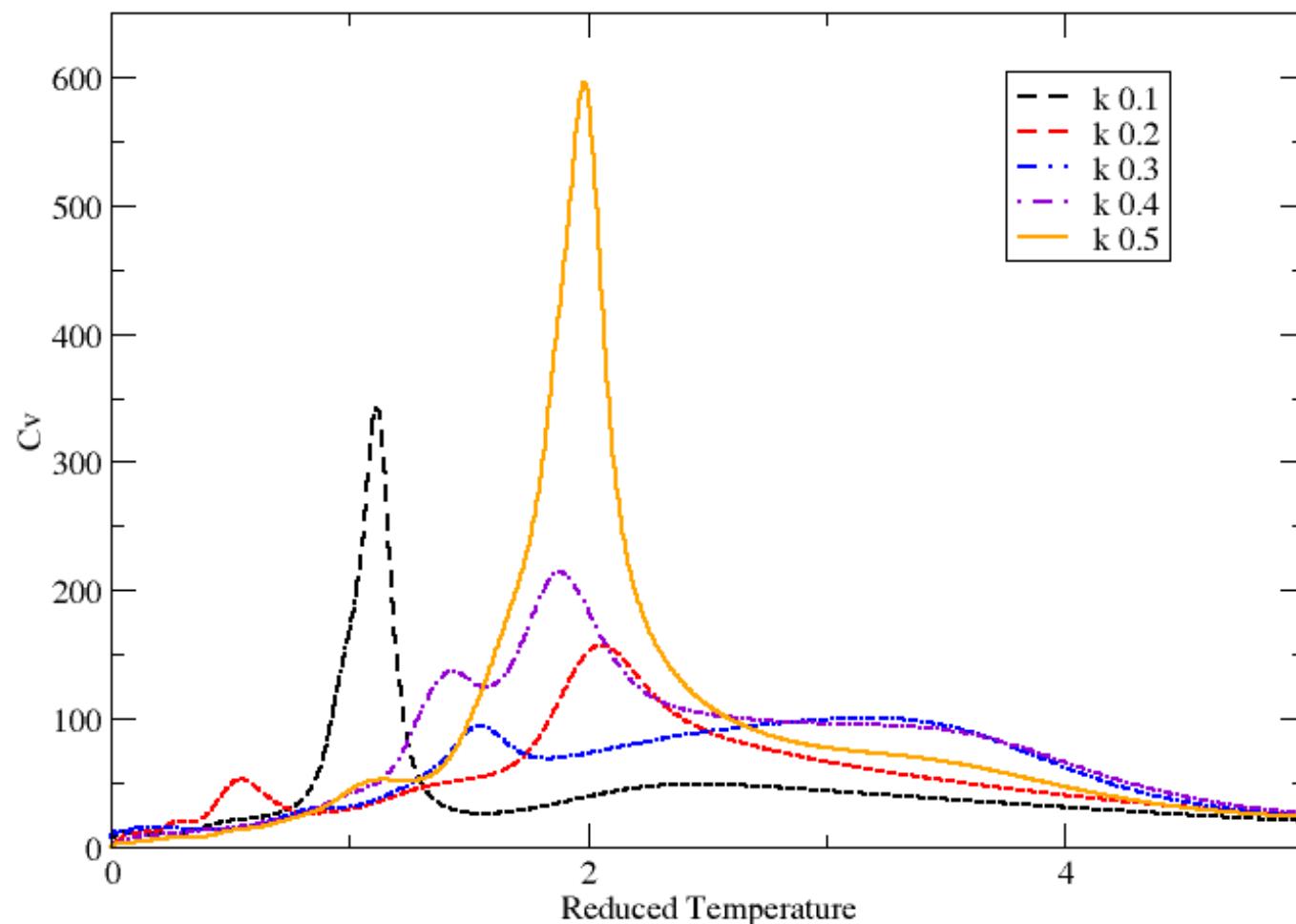
Average Heat Capacity of 4 Trials



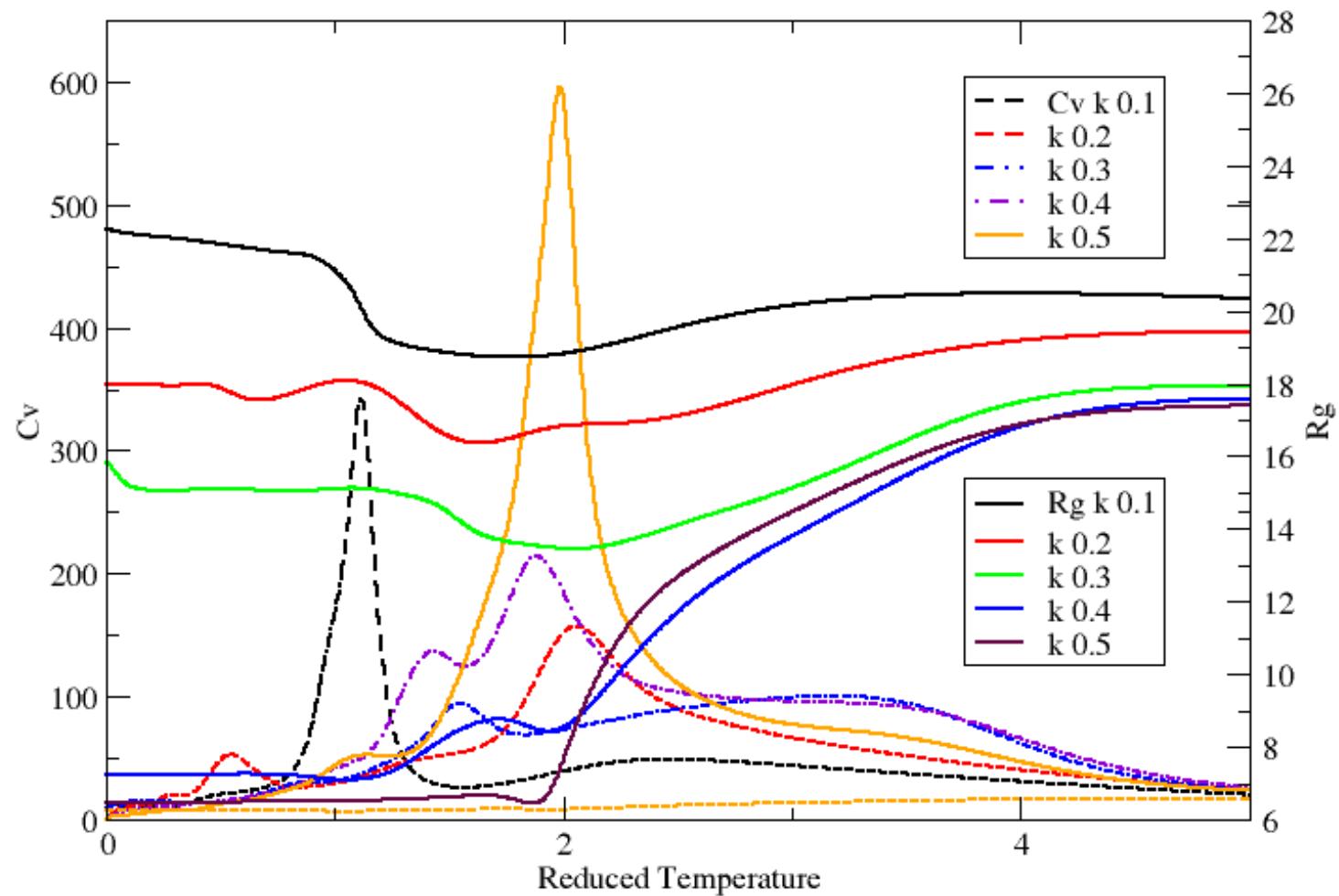
Average Heat Capacity of 4 Trials For each kappa value(0.1 – 1.0)



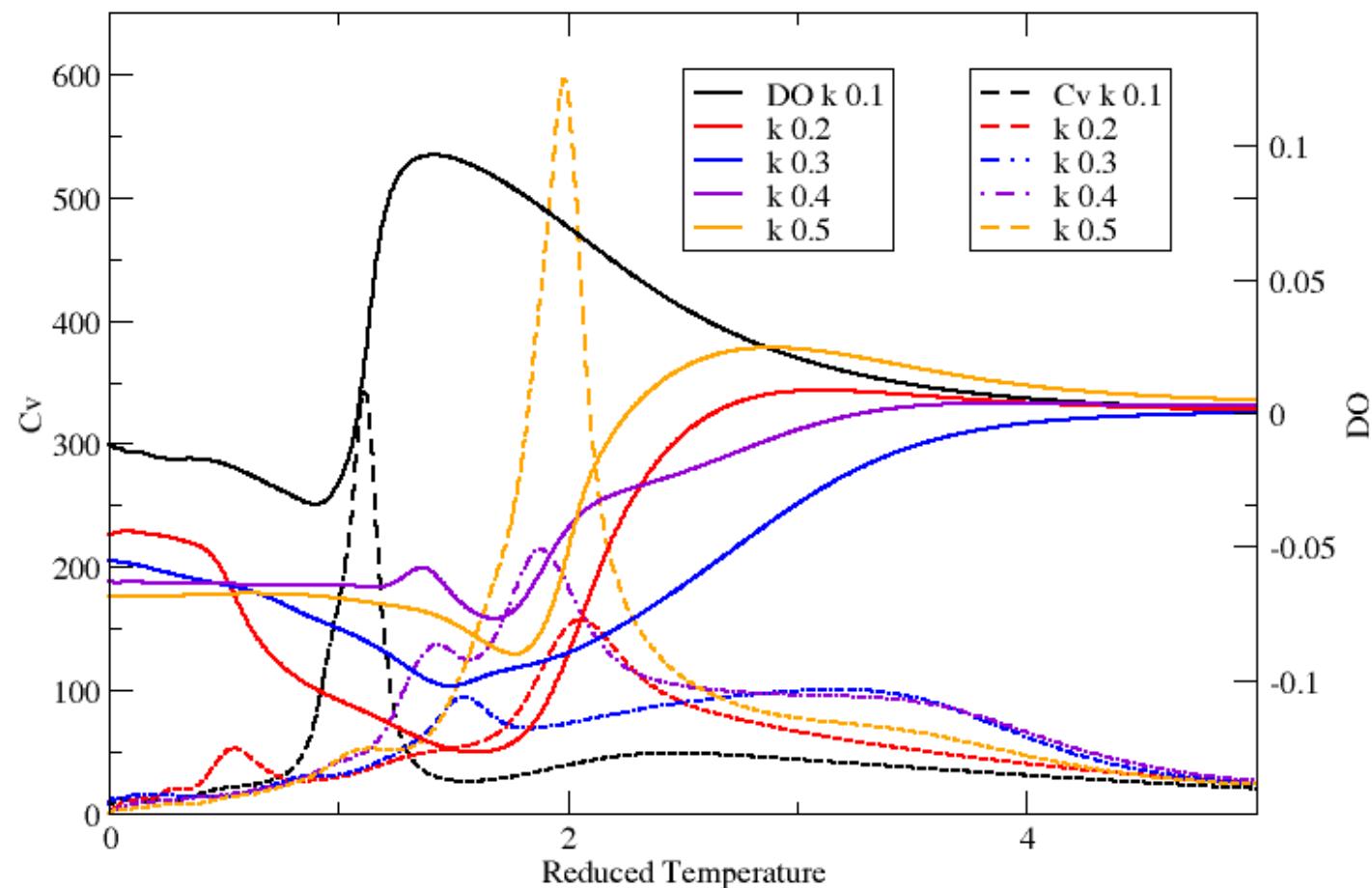
Average Heat Capacity of 4 Trials For each kappa value(0.1 – 0.5)



Overlayed average Cv and average Radius of Gyration(R_g) of for trials for kappa values(0.1-0.5)

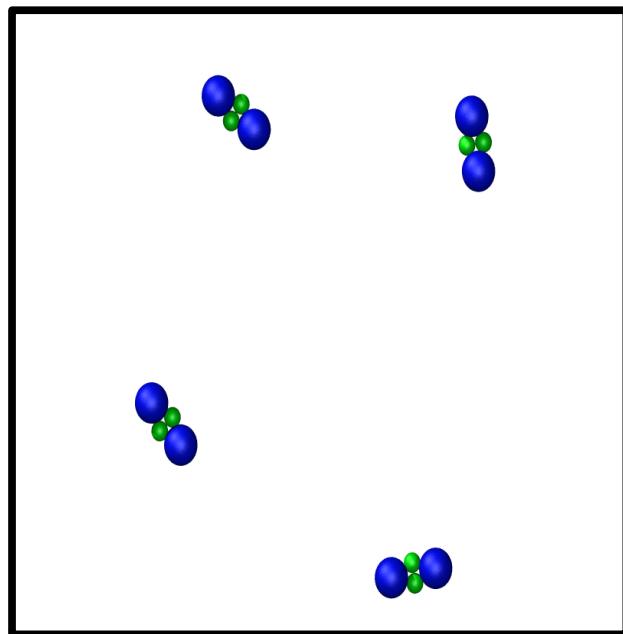


Overlayed average Cv and average Dimer-Dimer Orientation Order parameter (DO) of trials for kappa values(0.1-0.5)

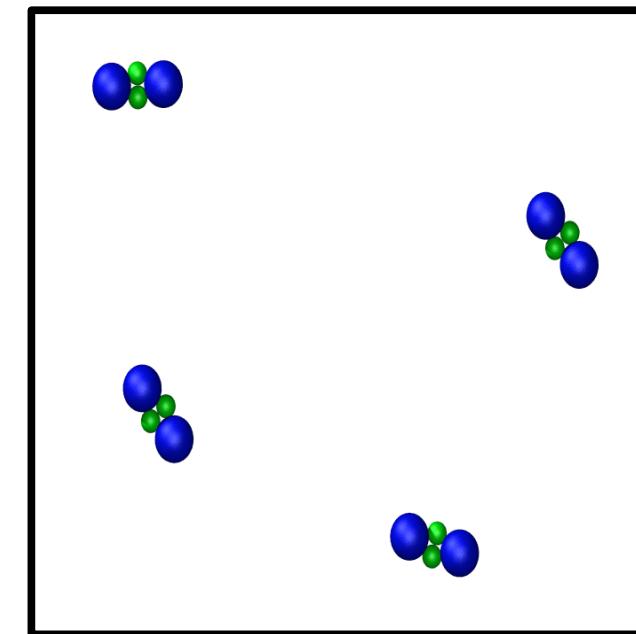


Kappa 0.15

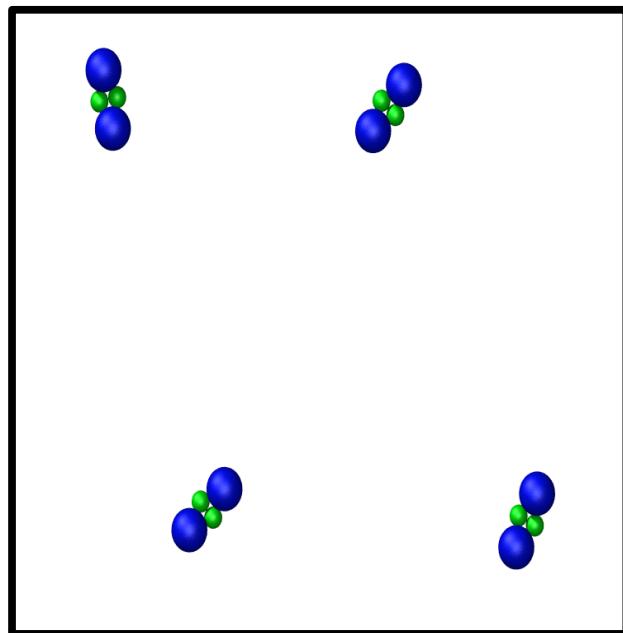
Lowest energy configuration sampled by each trial



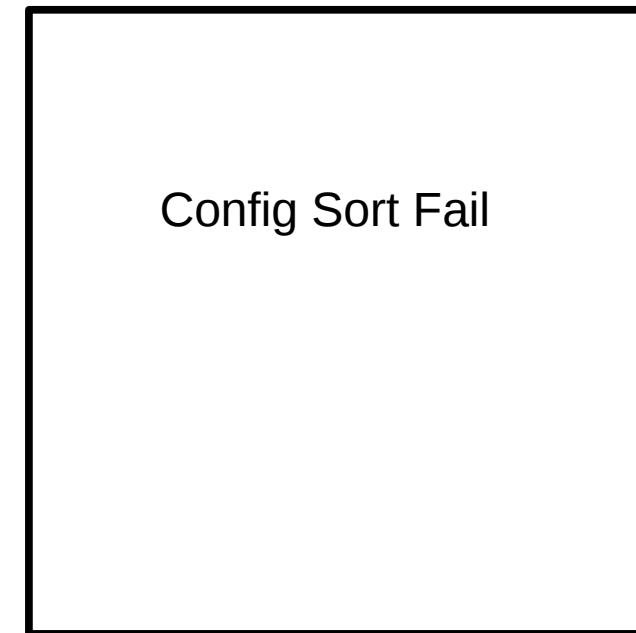
Trial1
 $E=-308.7763$



Trial2
 $E=-308.2958$



Trial3
 $E=-309.3333$

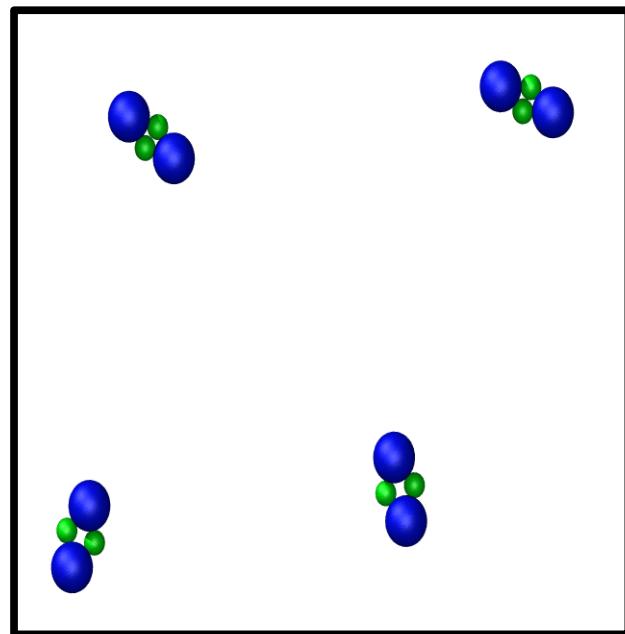


Trial4
 $E=$

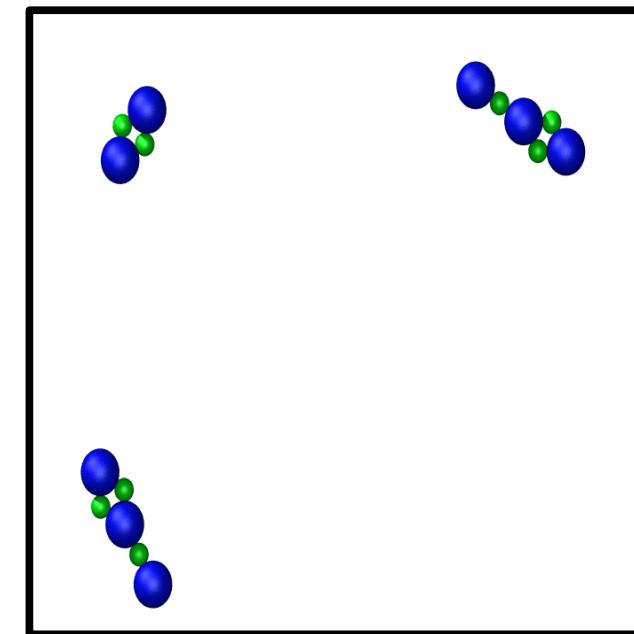
Config Sort Fail

Kappa 0.25

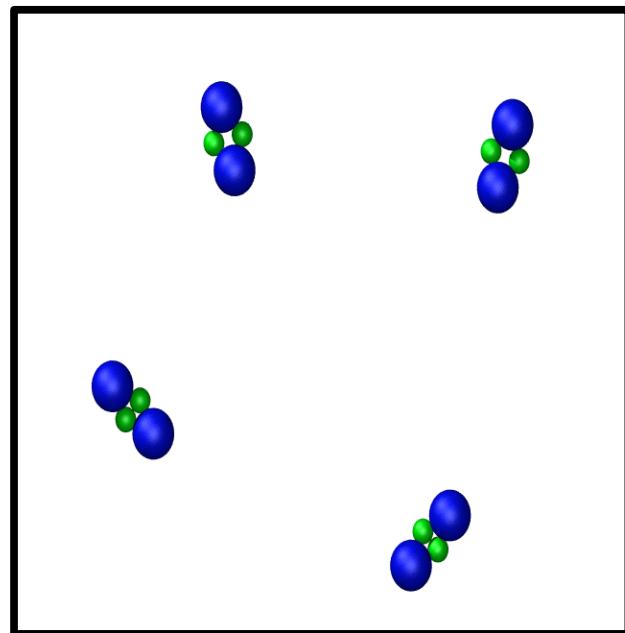
Lowest energy configuration sampled by each trial



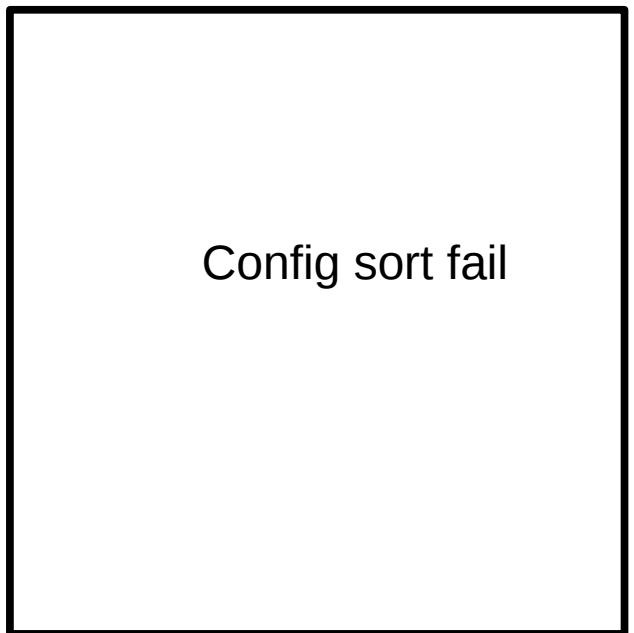
Trial1
 $E=-359.6198$



Trial2
 $E=-355.5539$



Trial3
 $E=-359.3452$

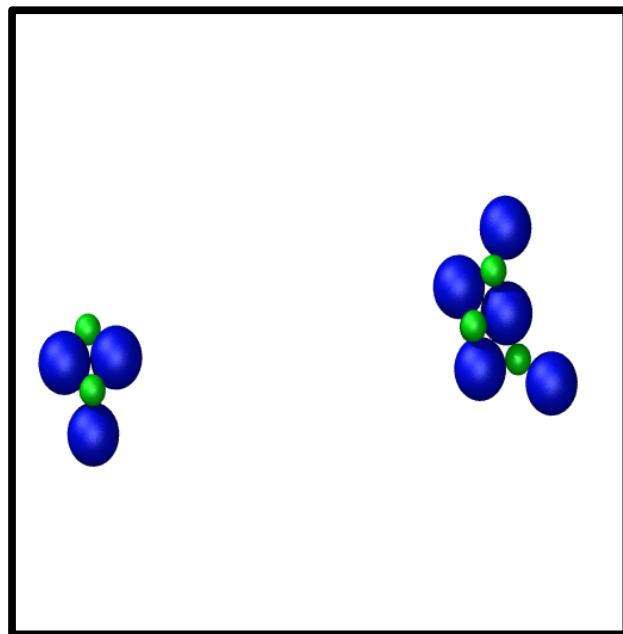


Trial4
 $E=$

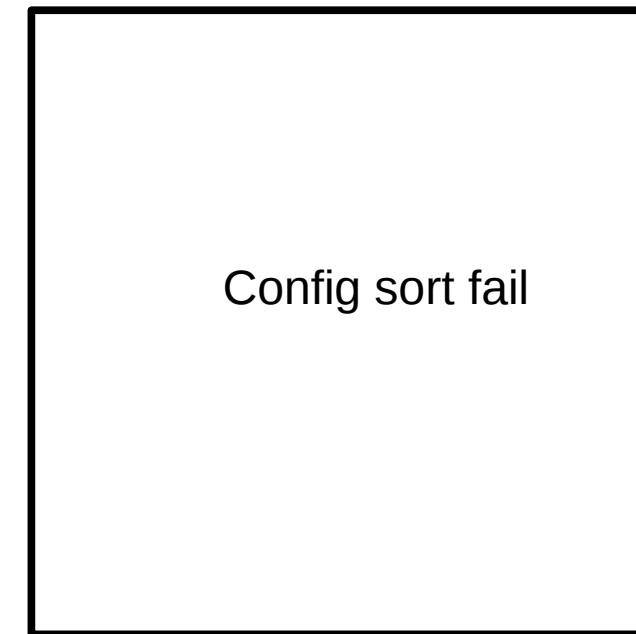
Config sort fail

Kappa 0.35

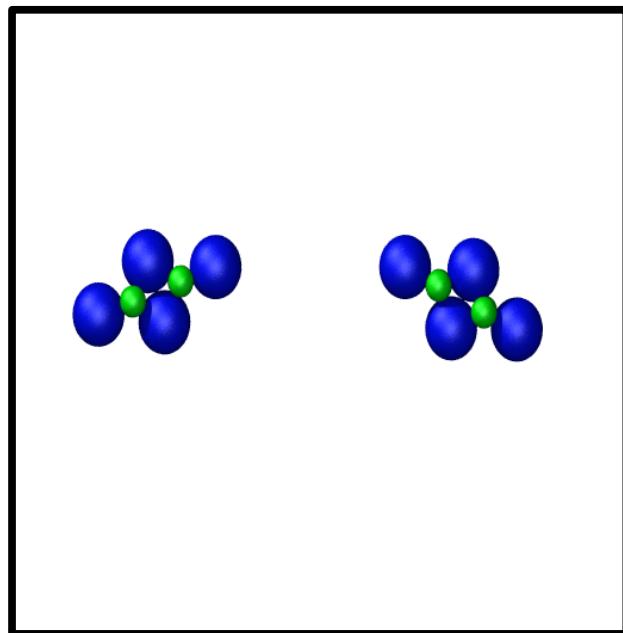
Lowest energy configuration sampled by each trial



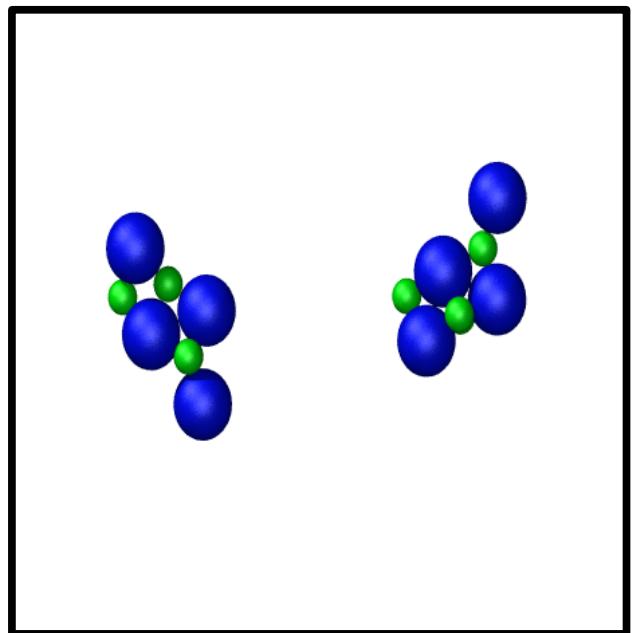
Trial1
 $E=-472.5265$



Trial2
 $E=$



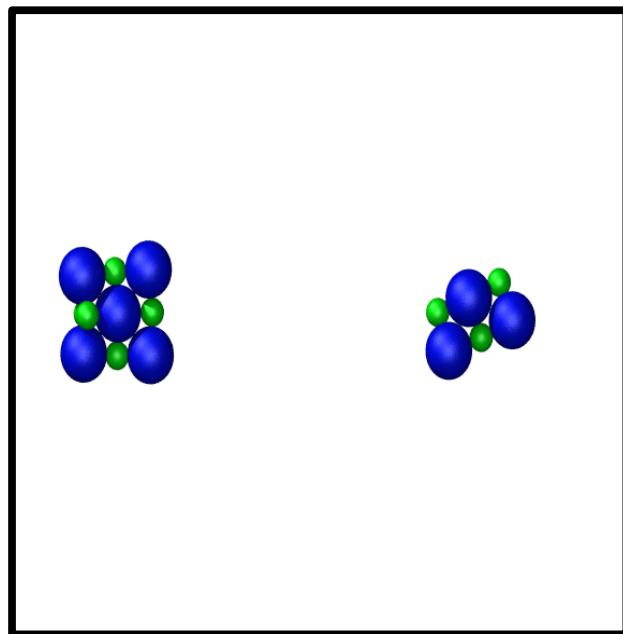
Trial3
 $E=-481.0048$



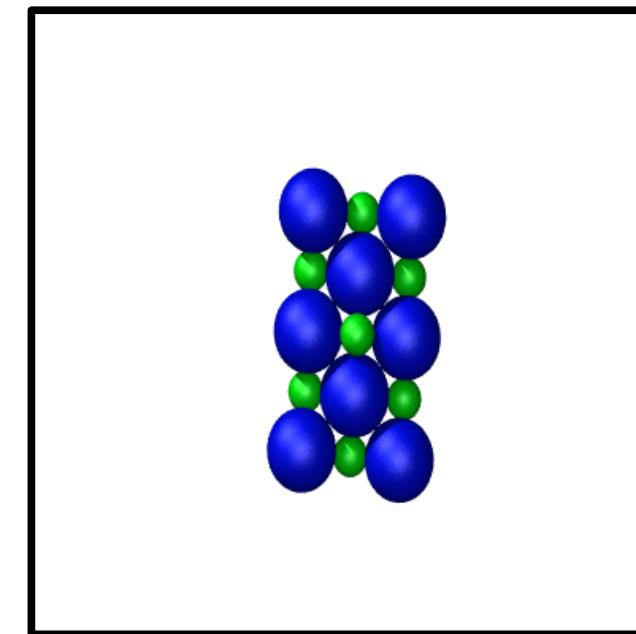
Trial4
 $E=-464.3097$

Kappa 0.45

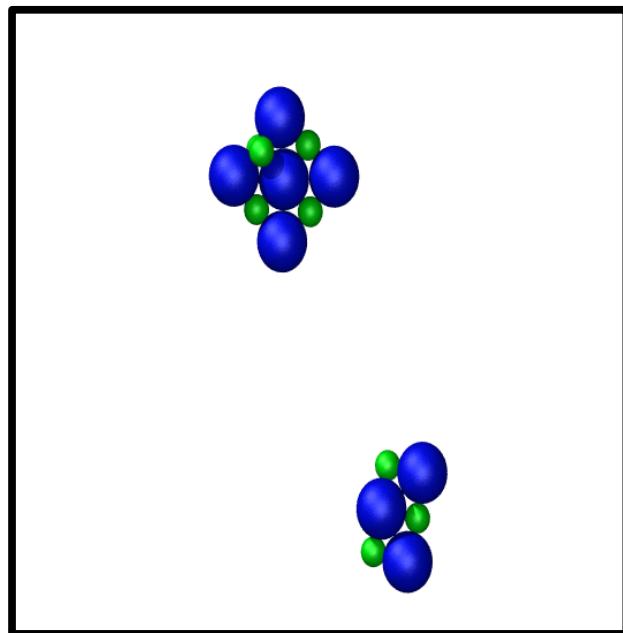
Lowest energy configuration sampled by each trial



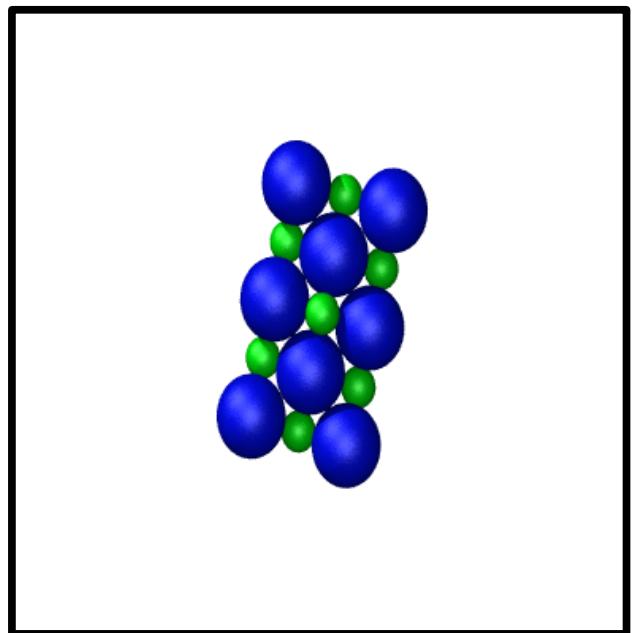
Trial1
 $E=-494.1081$



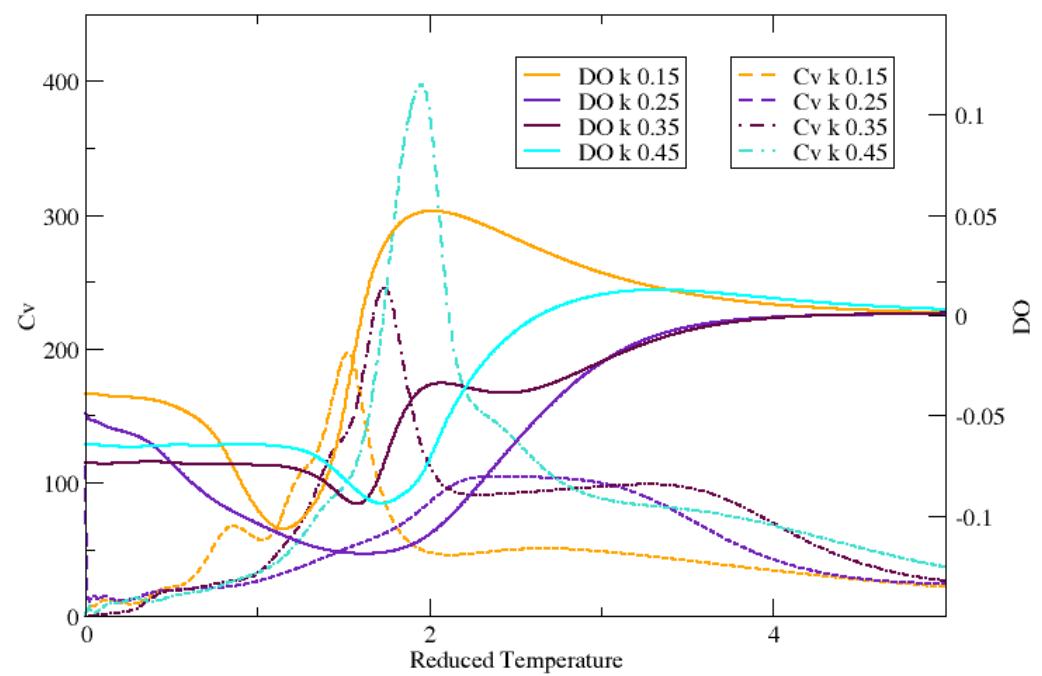
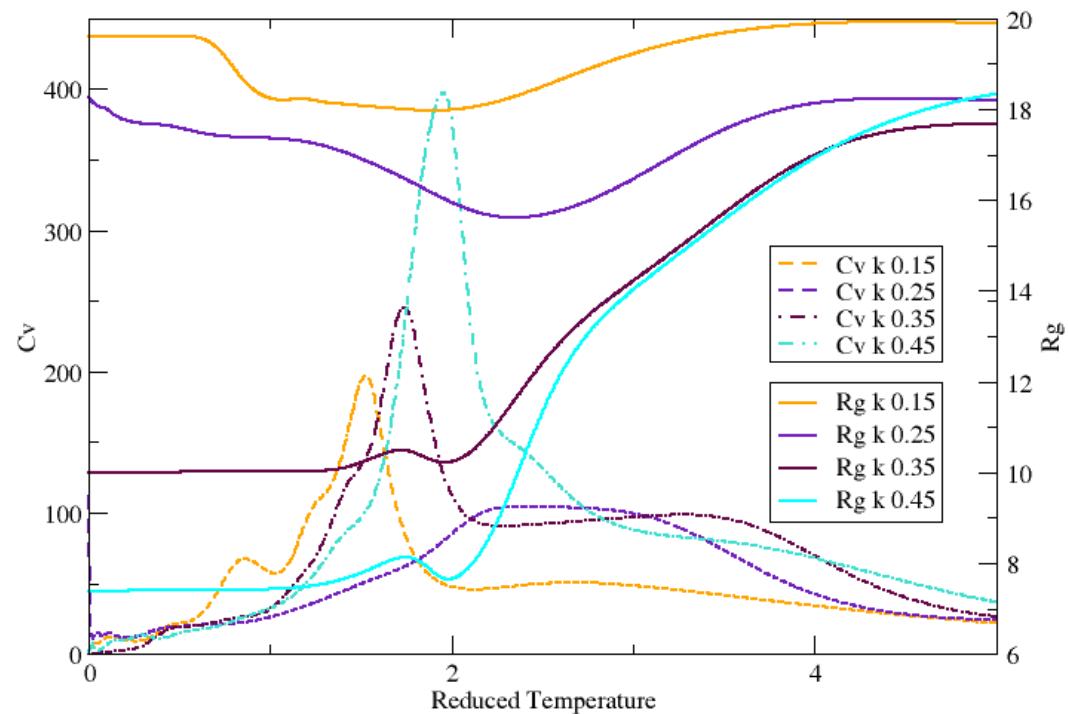
Trial2
 $E=-568.6315$



Trial3
 $E=-493.2773$



Trial4
 $E=-567.4456$



Dimer Parameters 2

$R_1 = 1.0$

$R_2 = 1.0$

$Ae_1 = 1000.0$

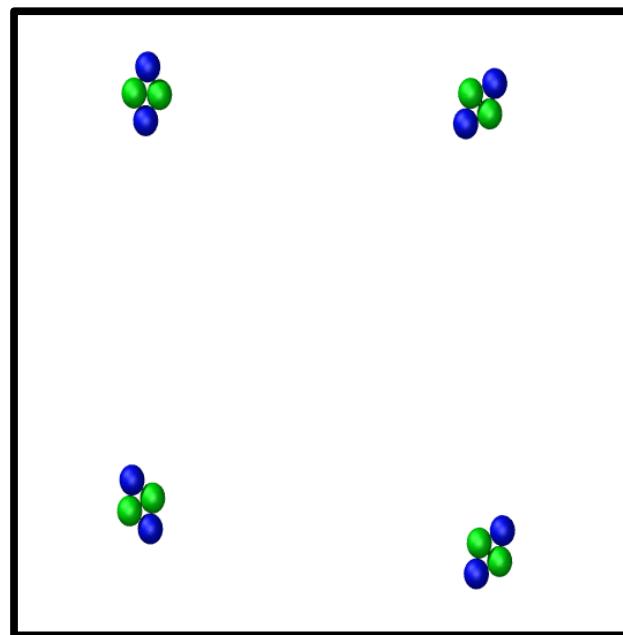
$Ae_2 = 5000.0$

$L_B = 2.0$

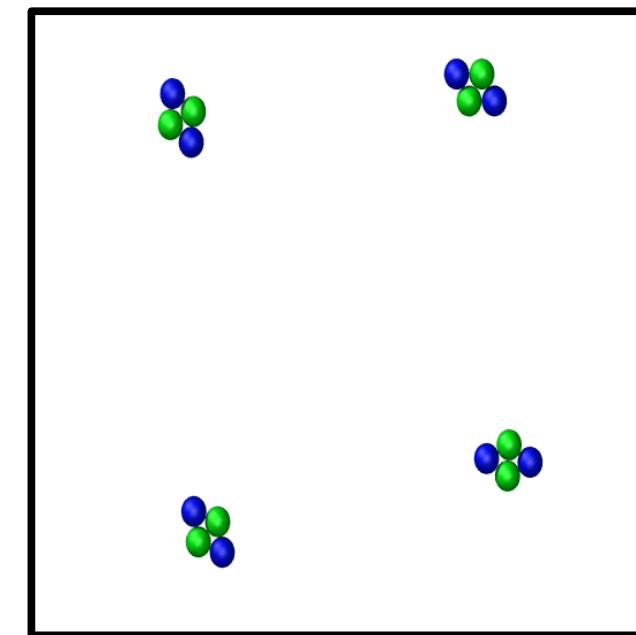
Ae values are the screened electrostatic energy-distance prefactor

Kappa 0.1

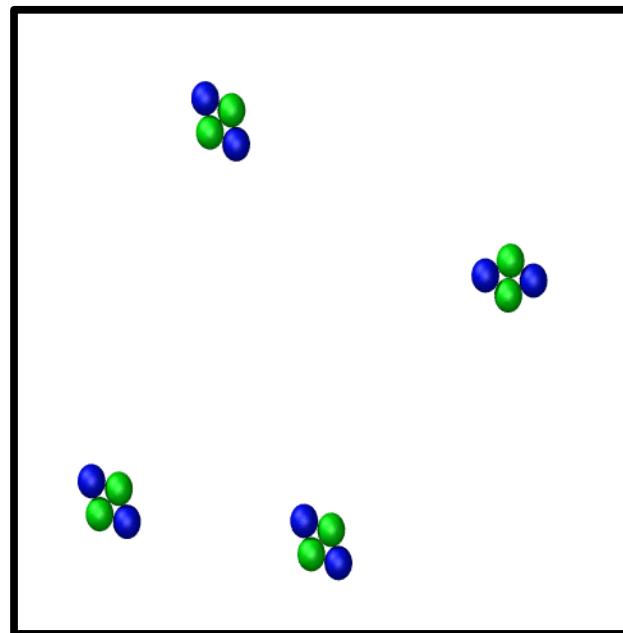
Lowest energy configuration sampled by each trial



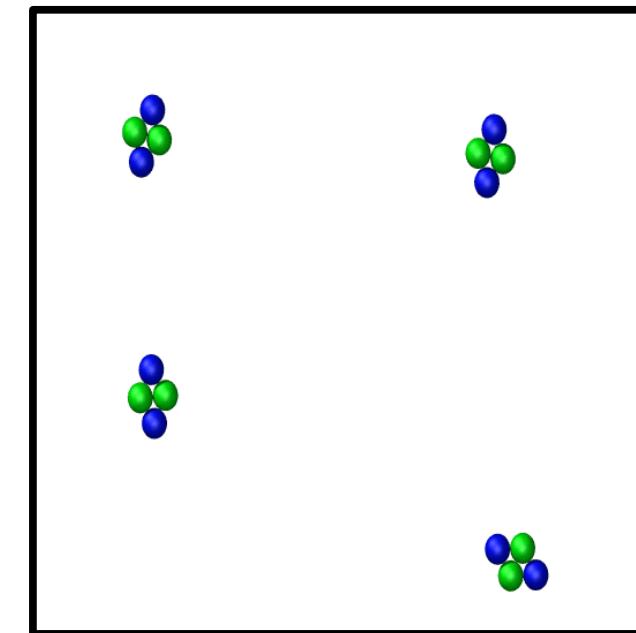
Trial1
 $E=-246.9533$



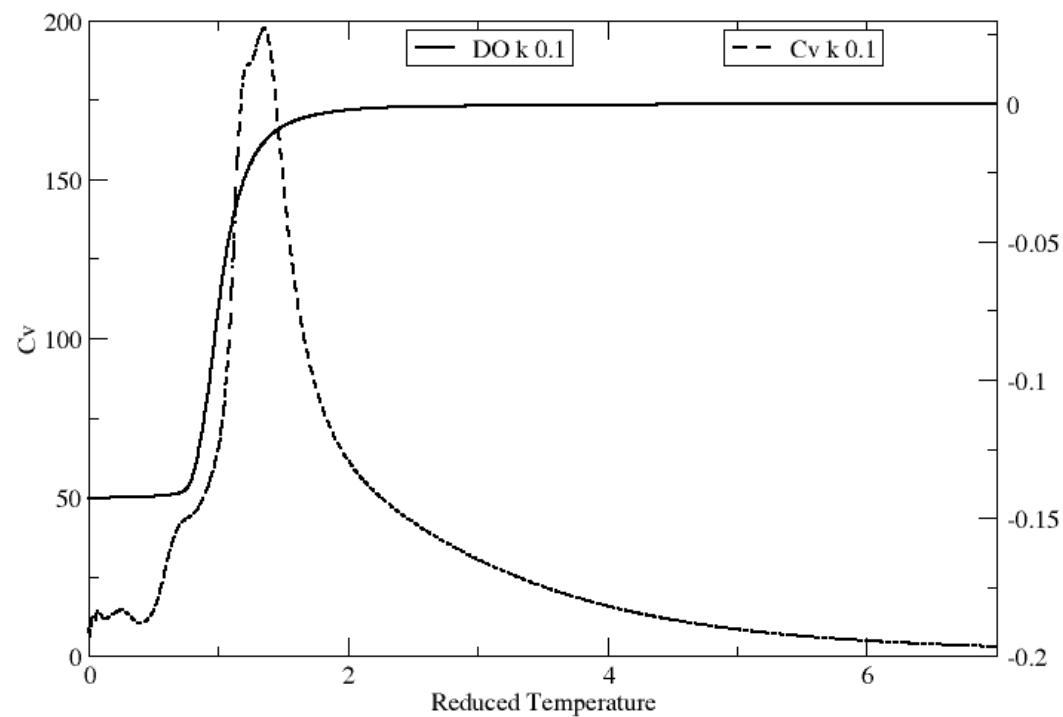
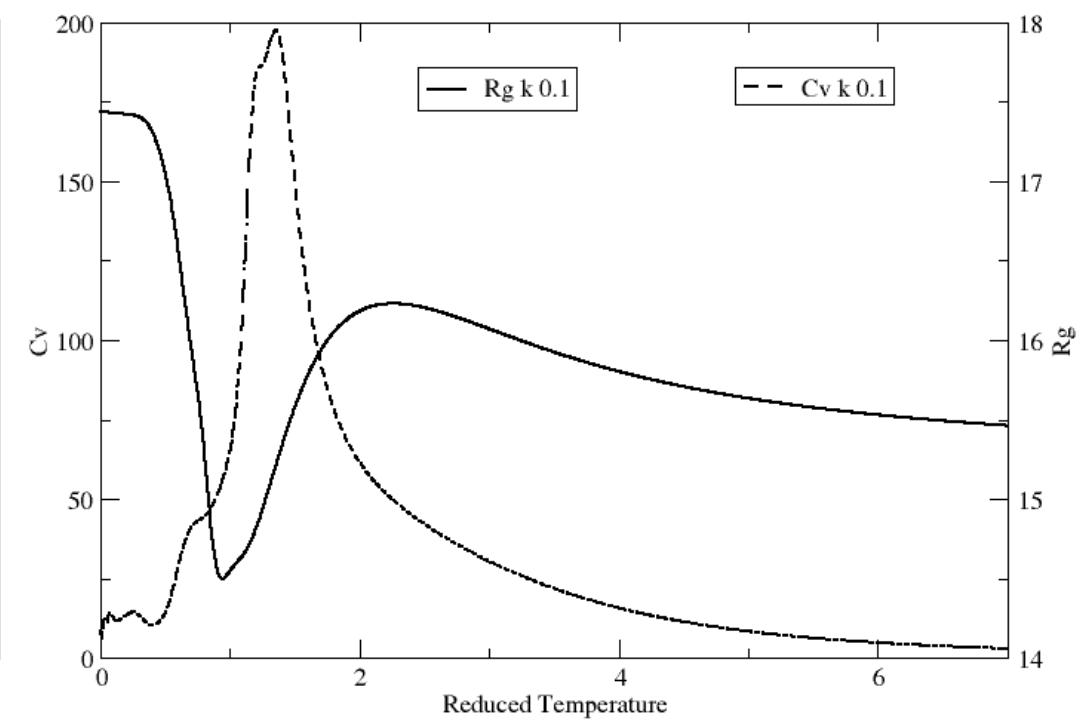
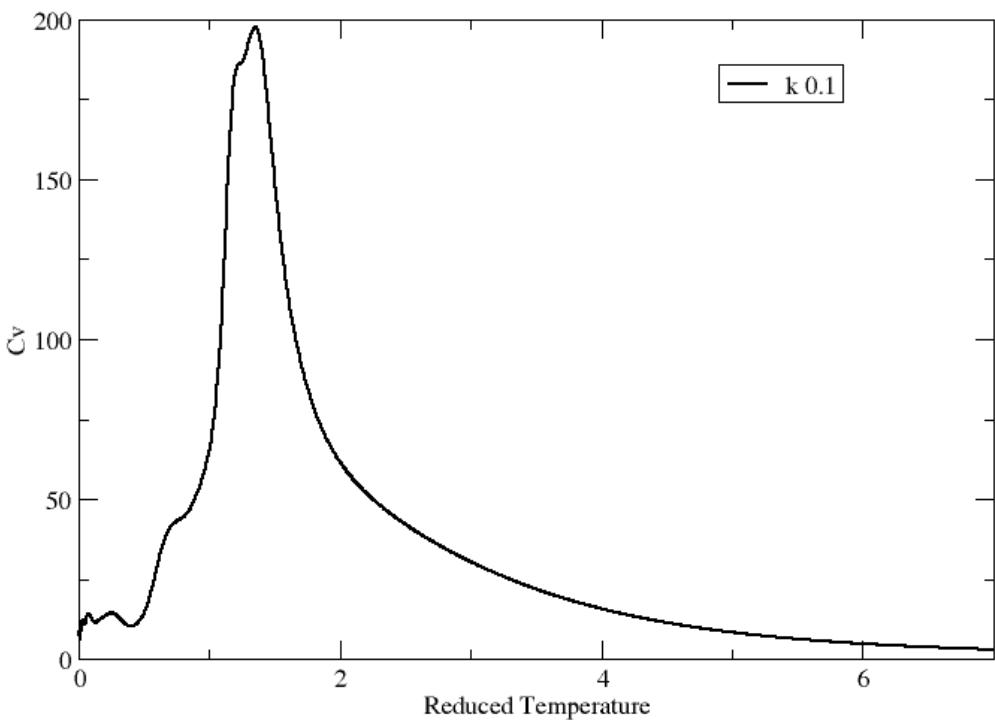
Trial2
 $E=-246.0730$



Trial3
 $E=-242.9574$

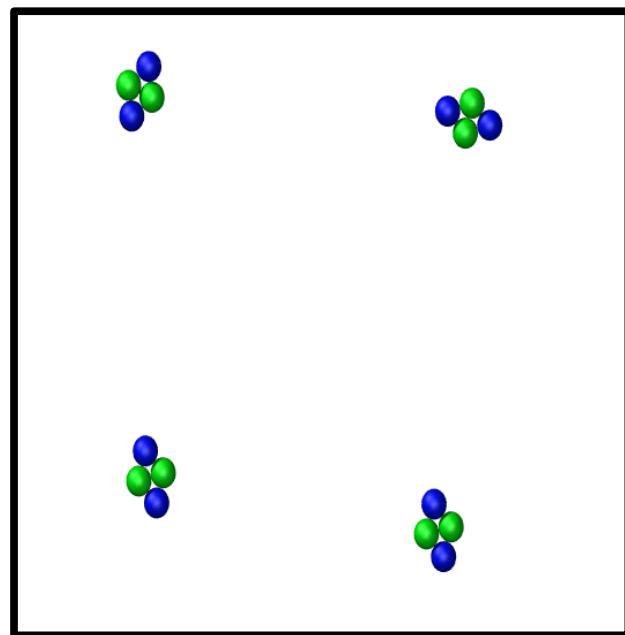


Trial4
 $E=-245.1638$

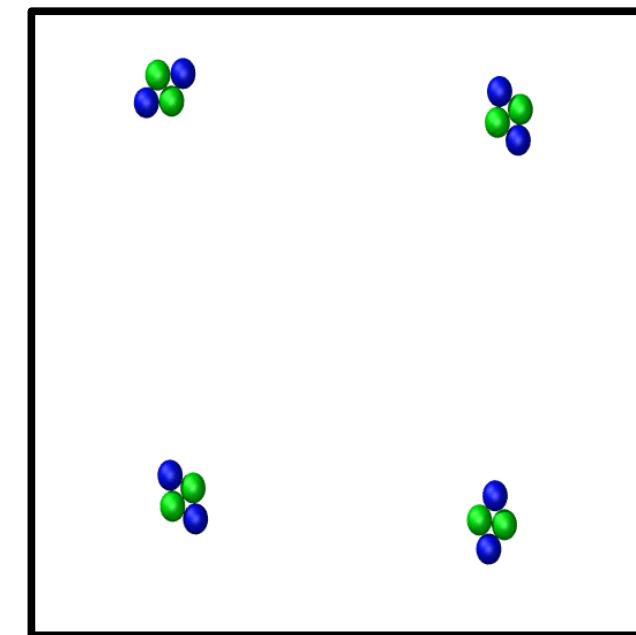


Kappa 0.15

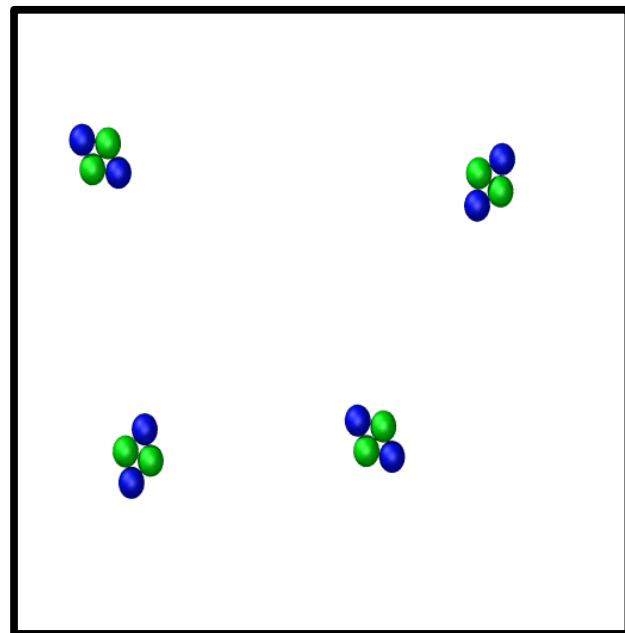
Lowest energy configuration sampled by each trial



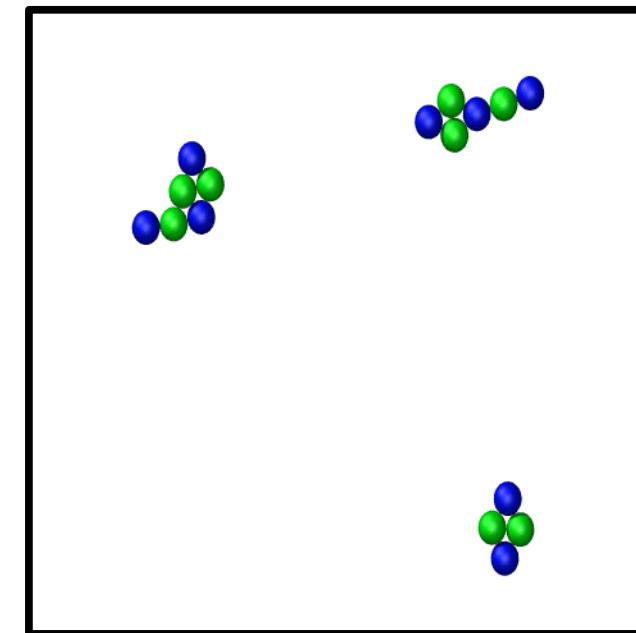
Trial1
 $E=-288.8223$



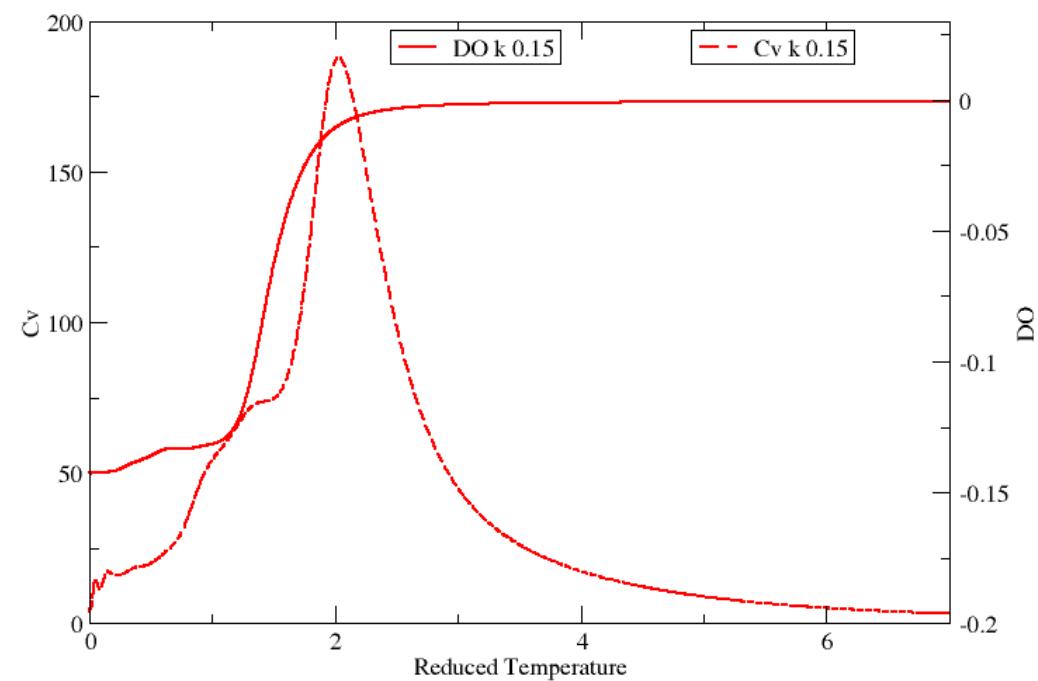
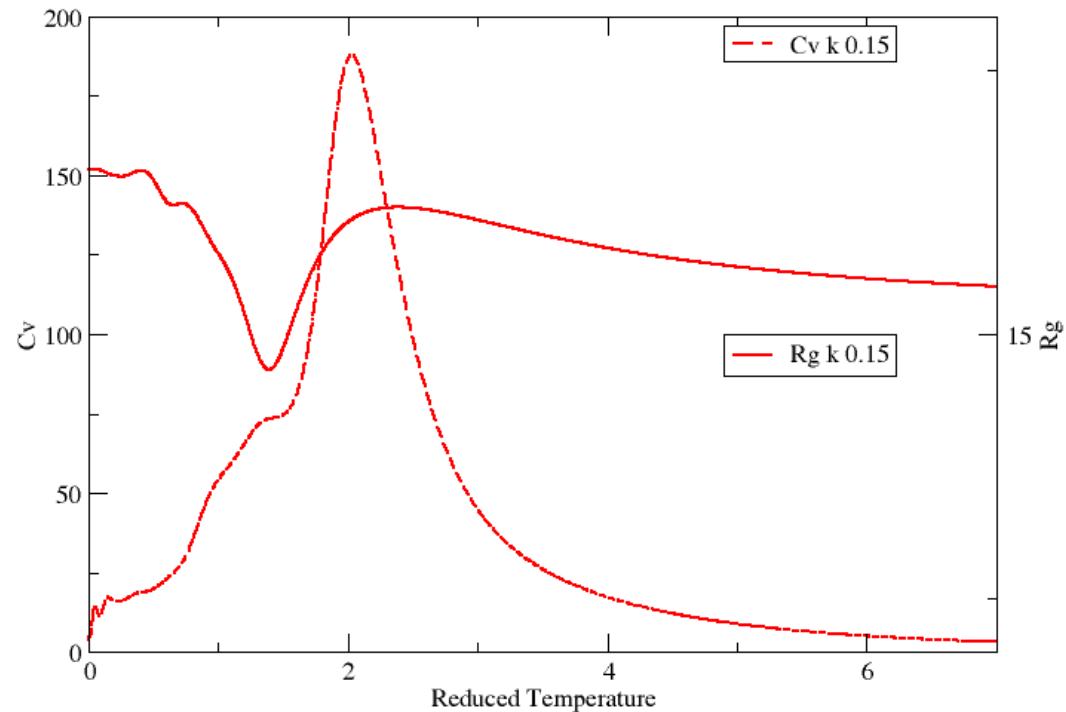
Trial2
 $E=-289.0675$



Trial3
 $E=-286.2671$

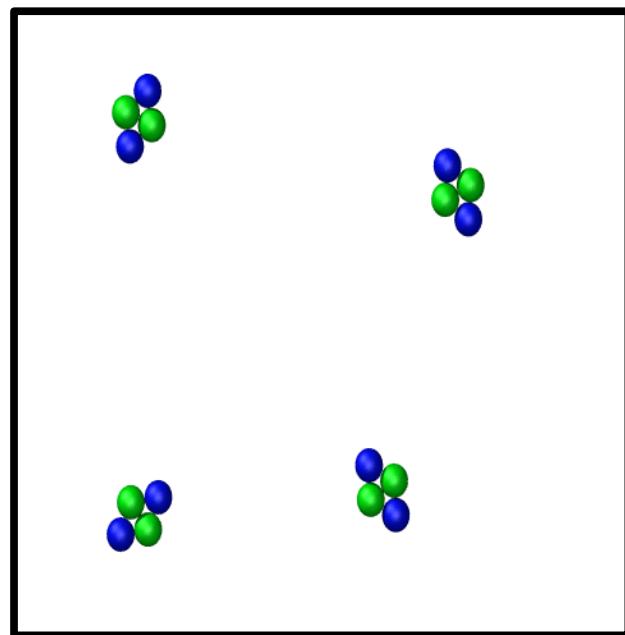


Trial4
 $E=-276.5522$

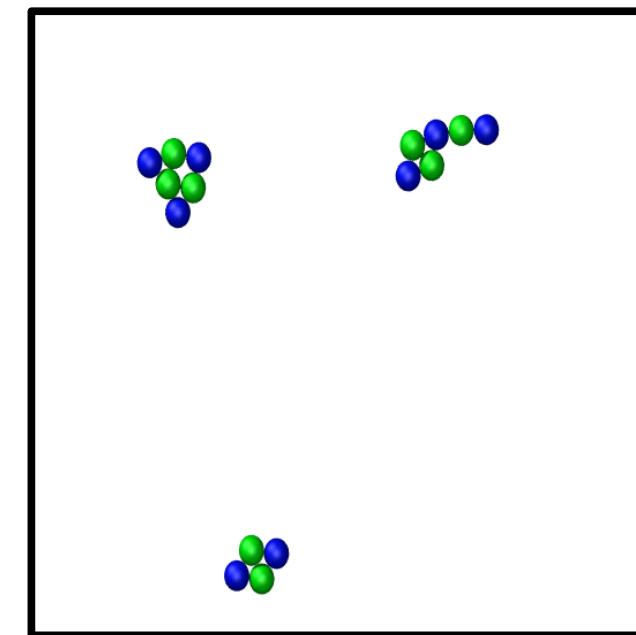


Kappa 0.2

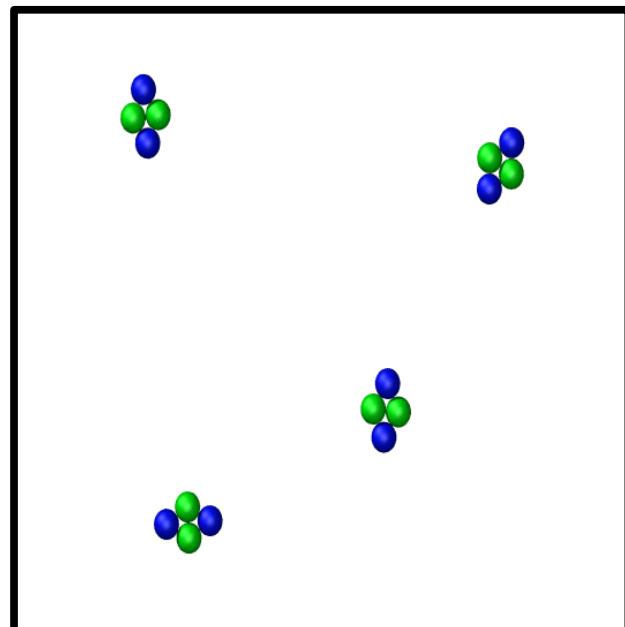
Lowest energy configuration sampled by each trial



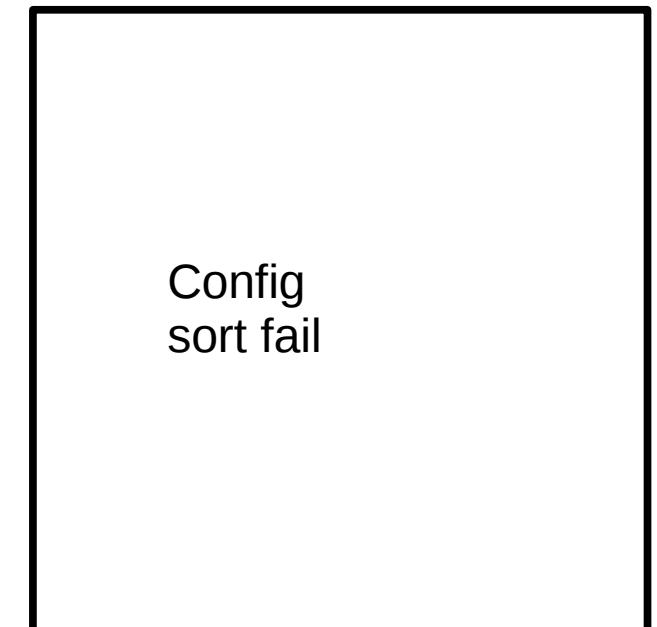
Trial1
 $E=-331.0455$



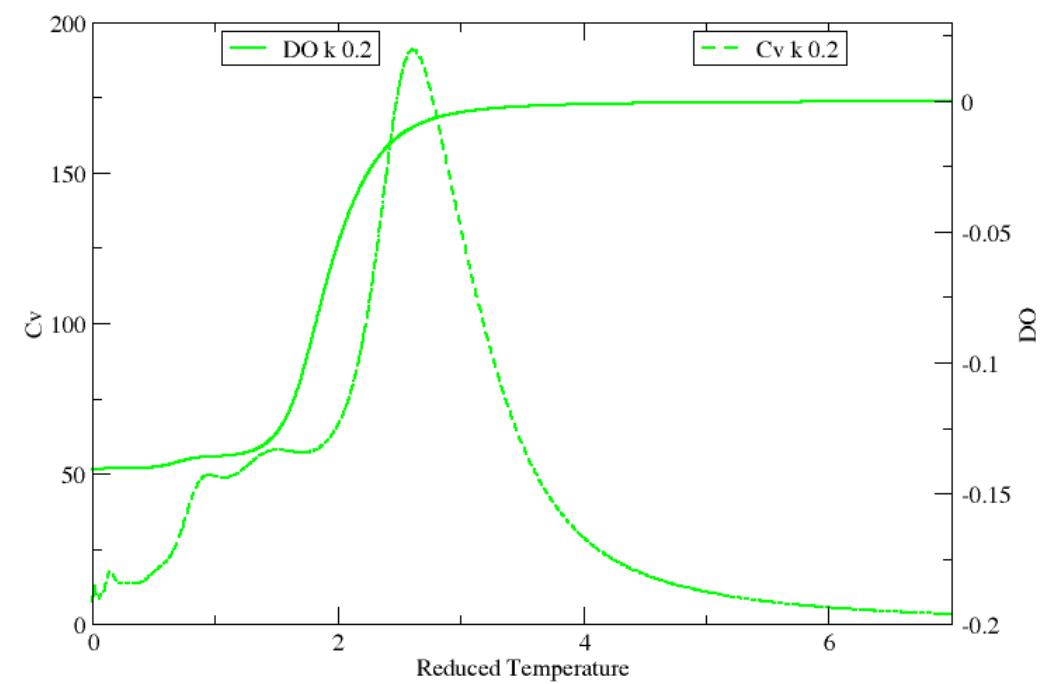
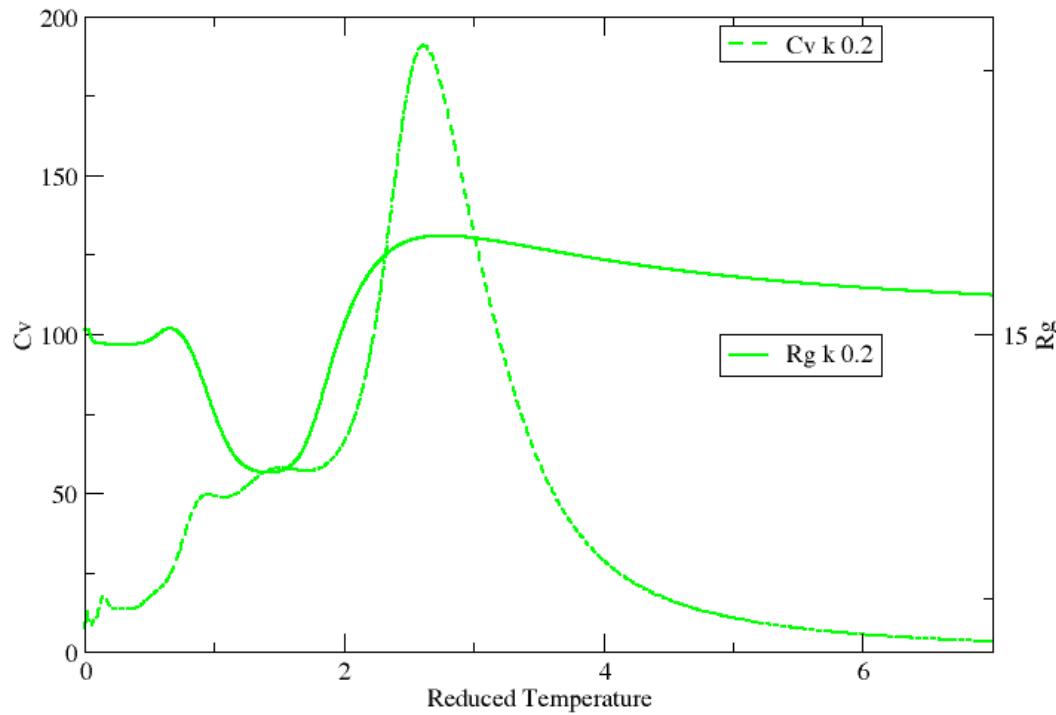
Trial2
 $E=-321.9488$



Trial3
 $E=-331.0624$

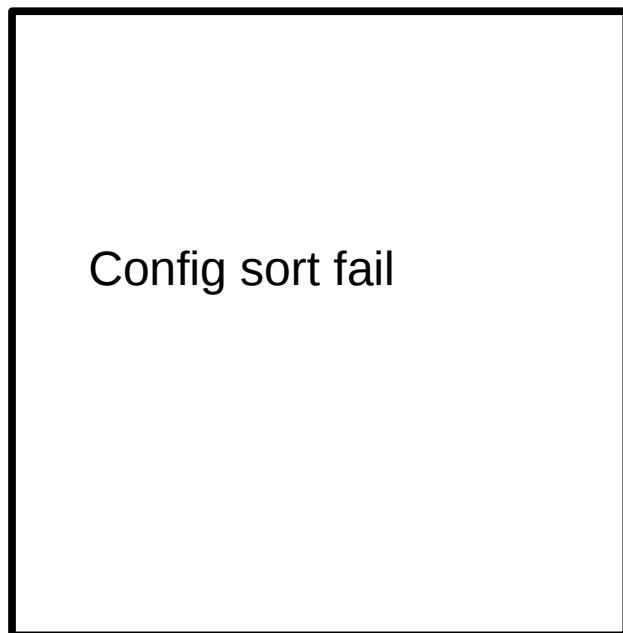


Trial4
 $E=$



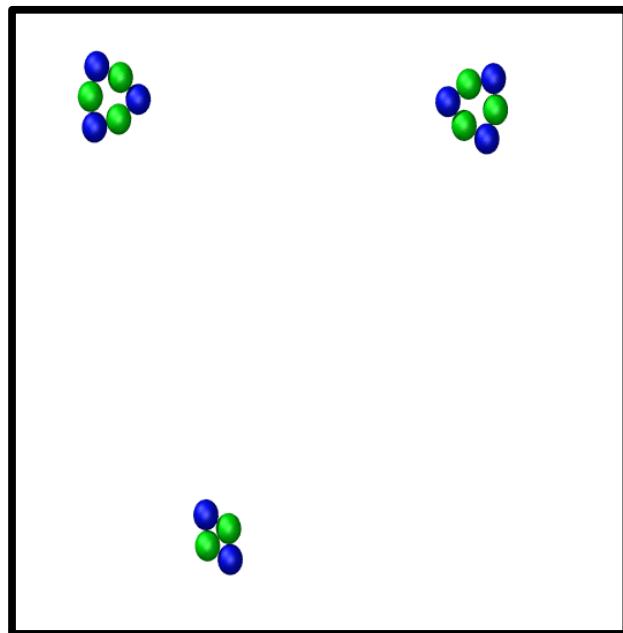
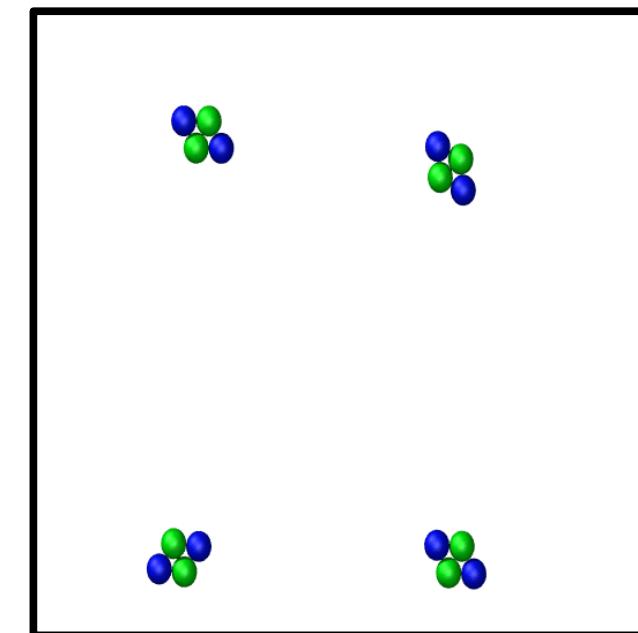
Kappa 0.25

Lowest energy configuration sampled by each trial



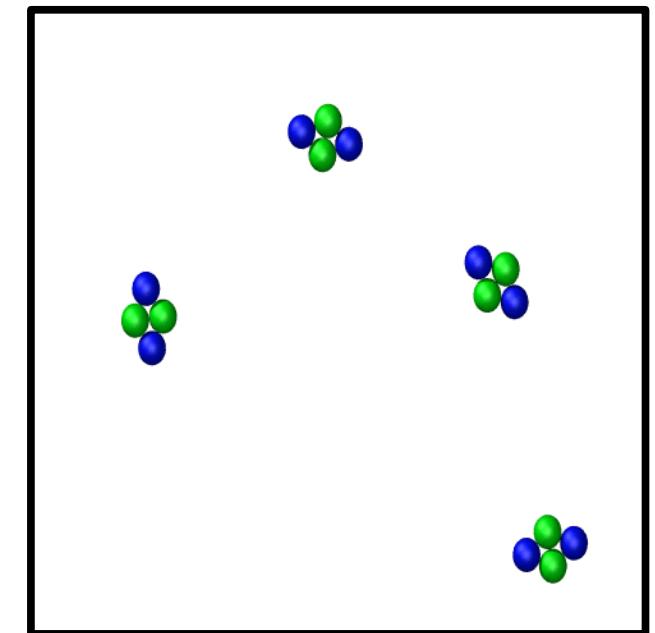
Trial1
 $E =$

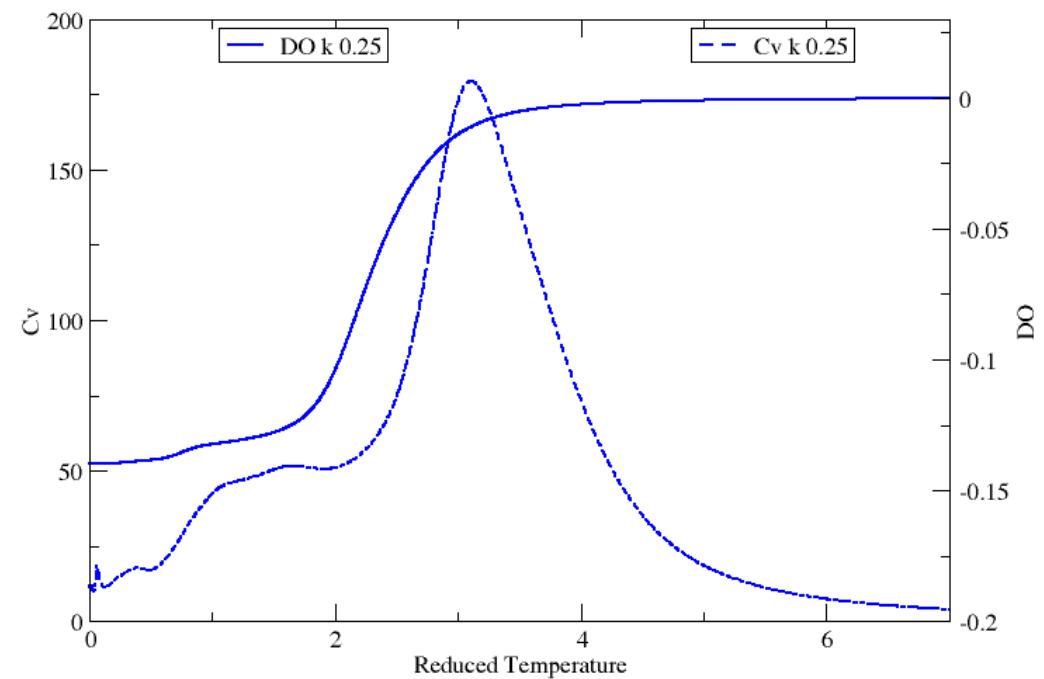
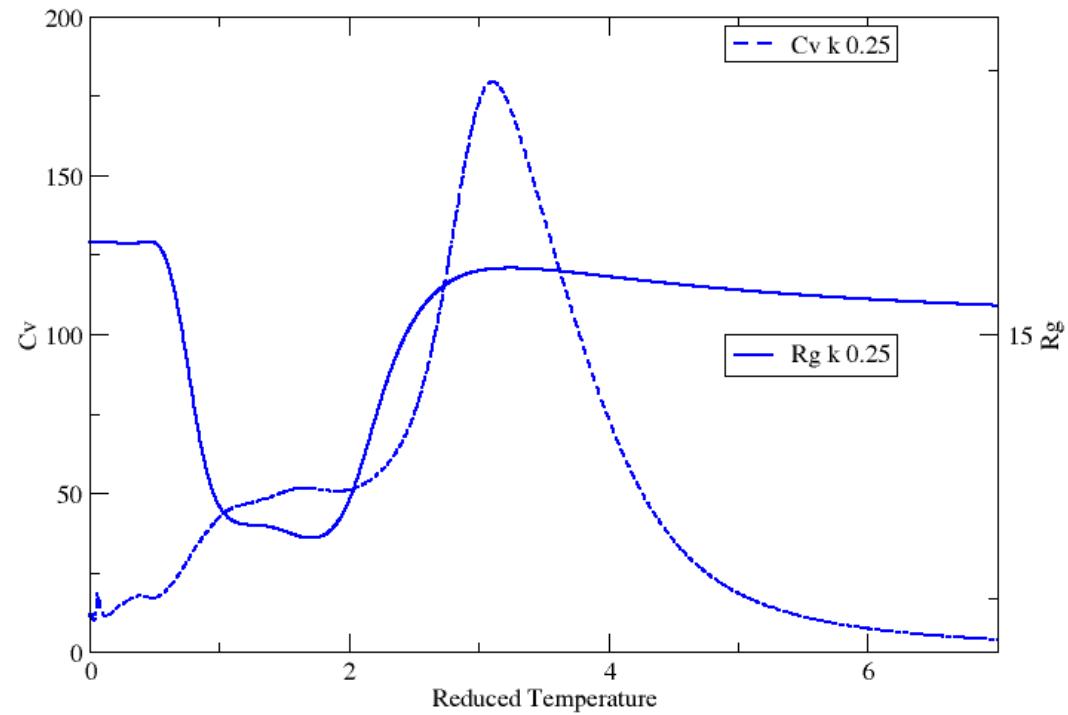
Trial2
 $E = -370.8267$



Trial3
 $E = -360.3559$

Trial4
 $E = -368.3916$





Kappa 0.3

Lowest energy configuration sampled by each trial

Config sort fail

Trial1

$E =$



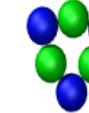
Trial2

$E = -395.9756$



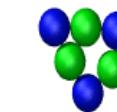
Trial3

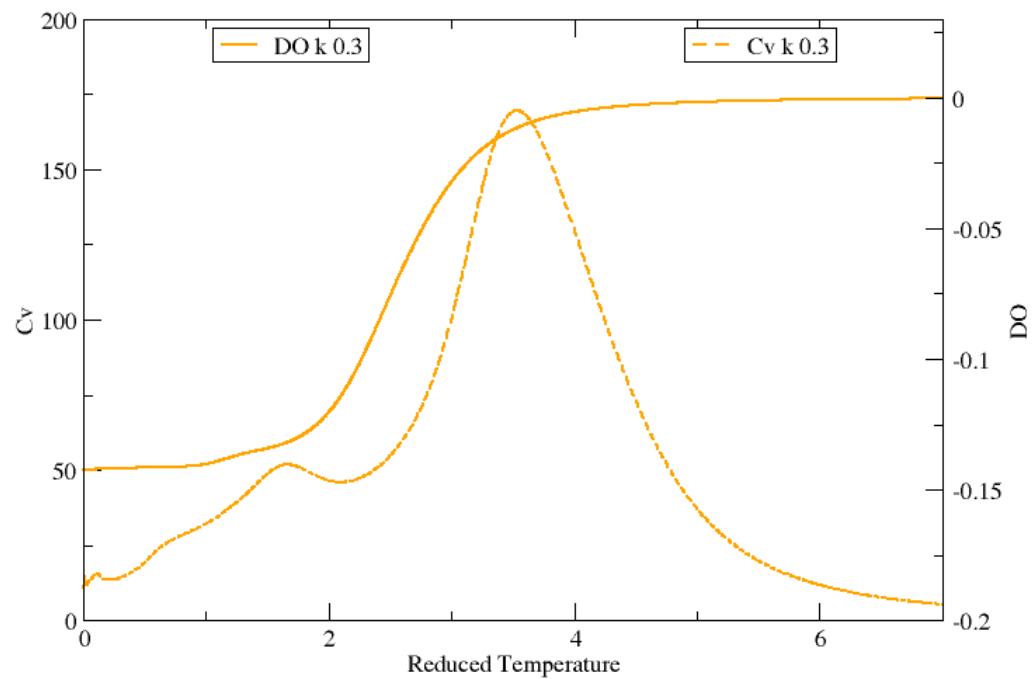
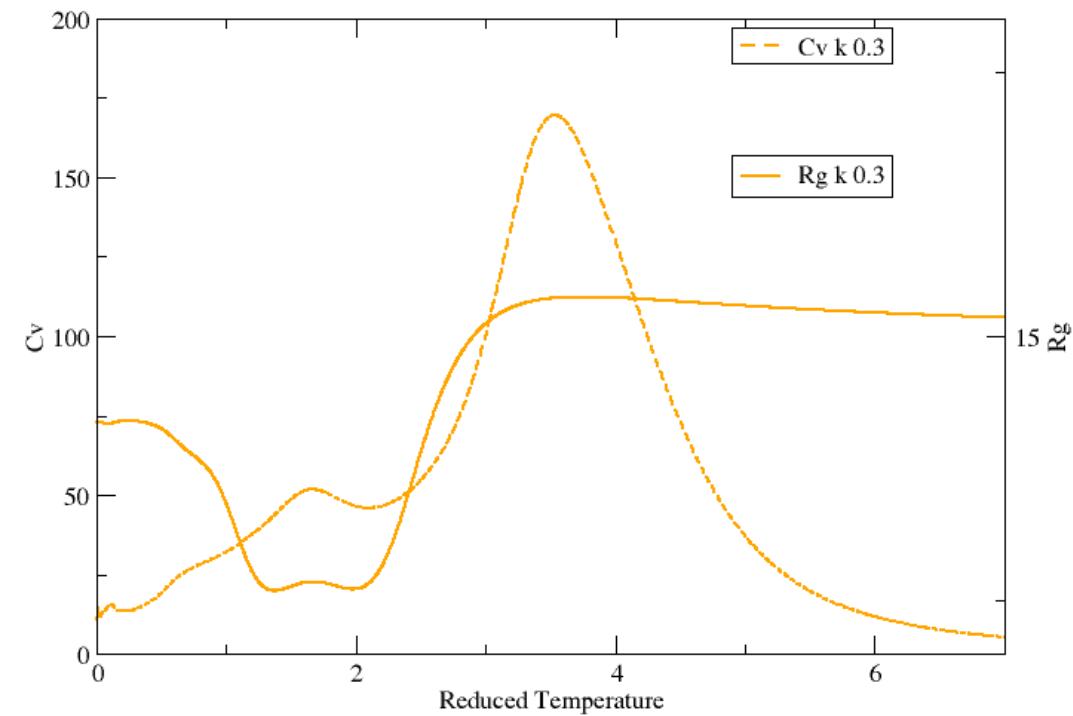
$E = -399.9042$



Trial4

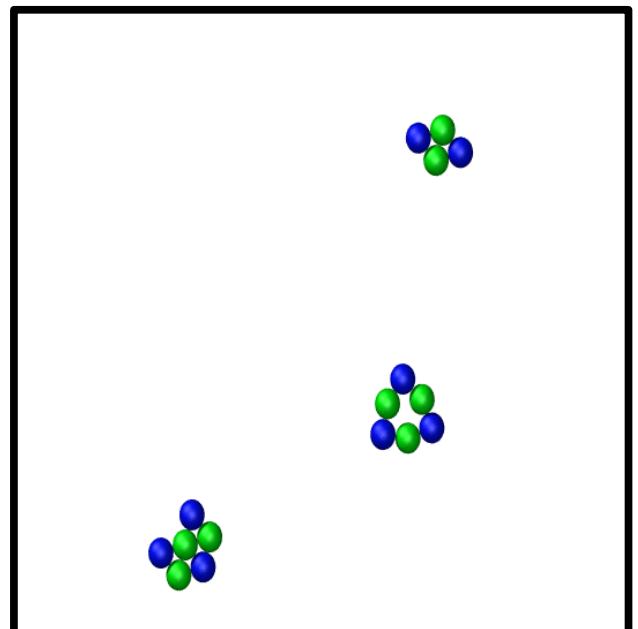
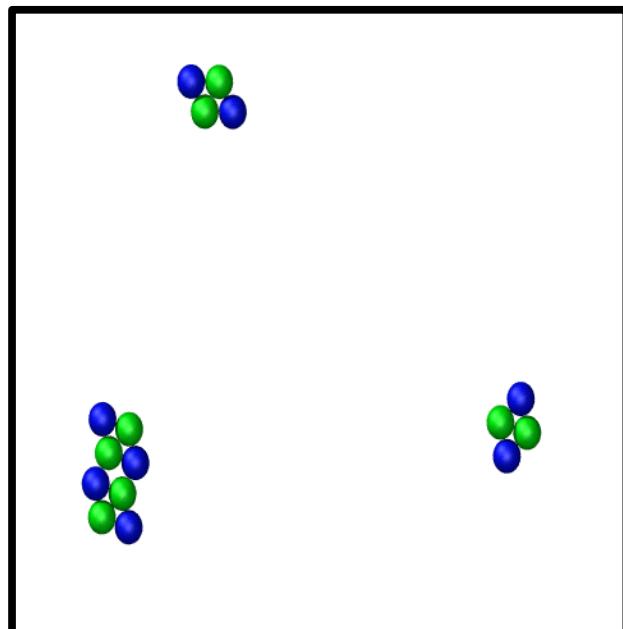
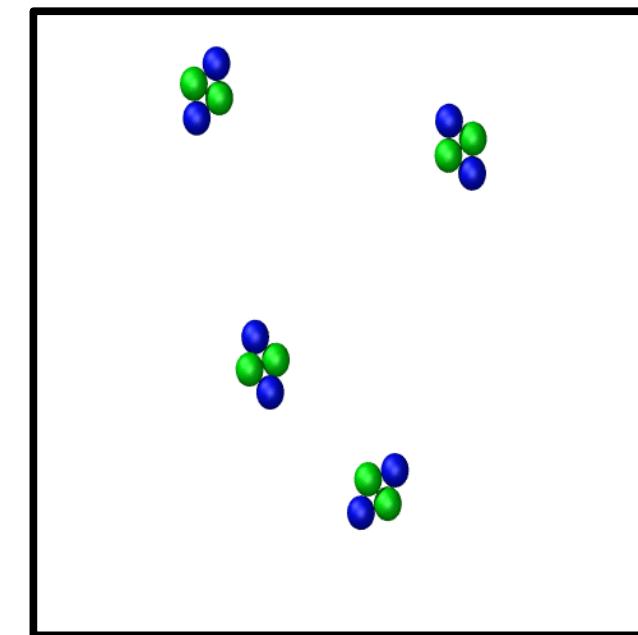
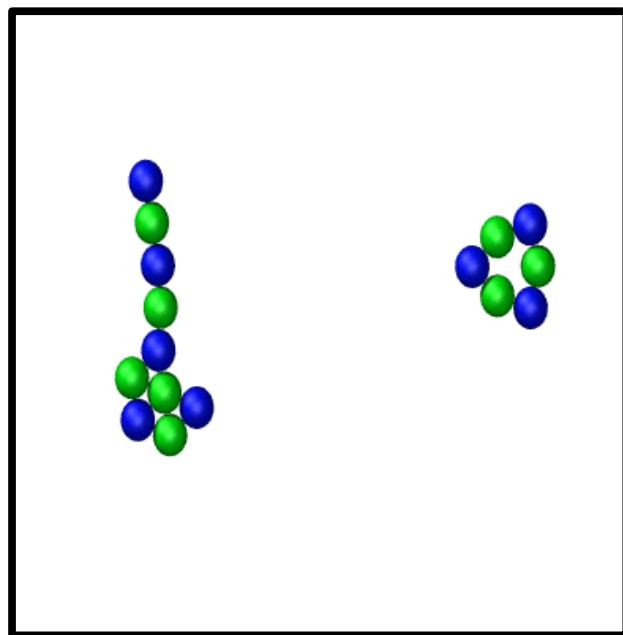
$E = -395.8685$

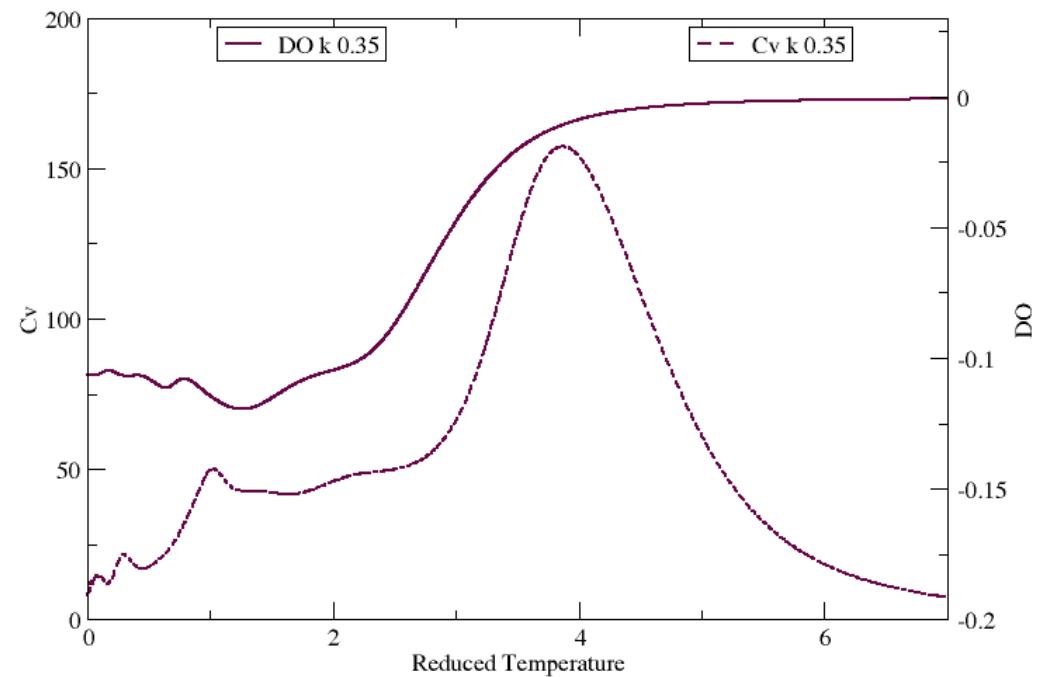
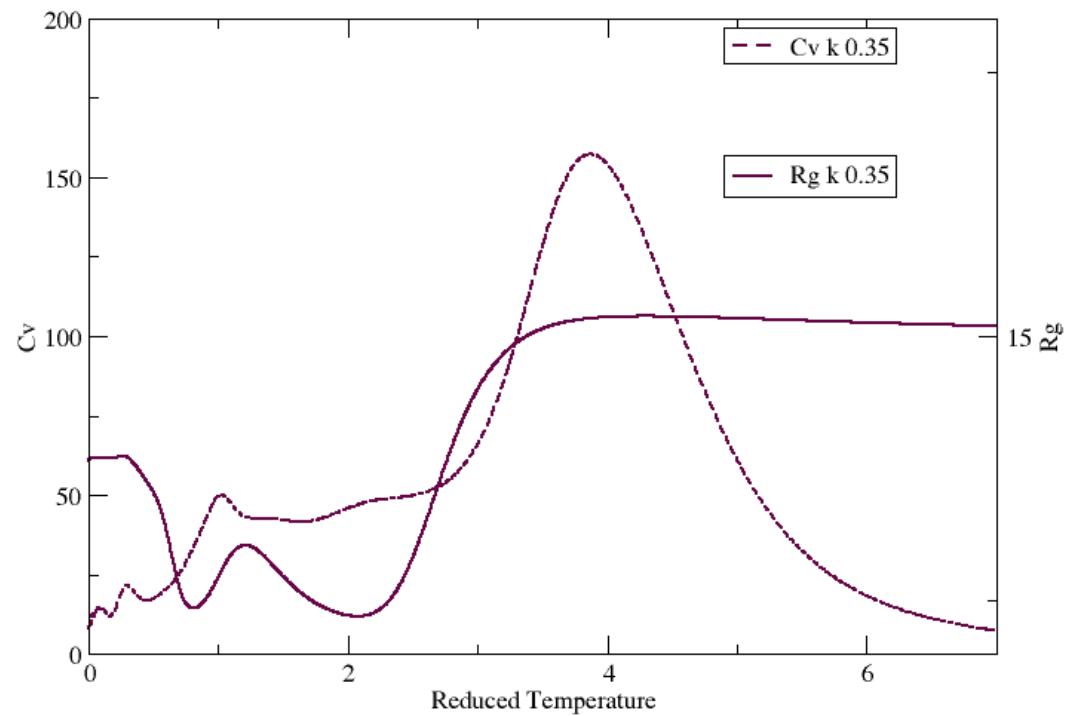




Kappa 0.35

Lowest energy configuration sampled by each trial



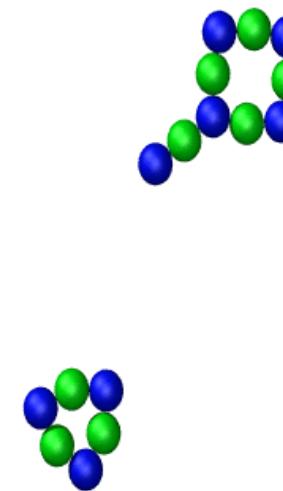


Kappa 0.4

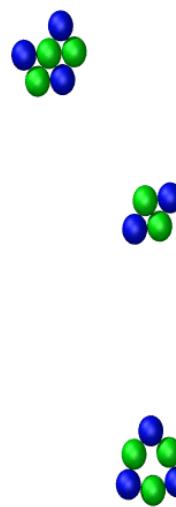
Lowest energy configuration sampled by each trial



Trial1
 $E=-442.5273$



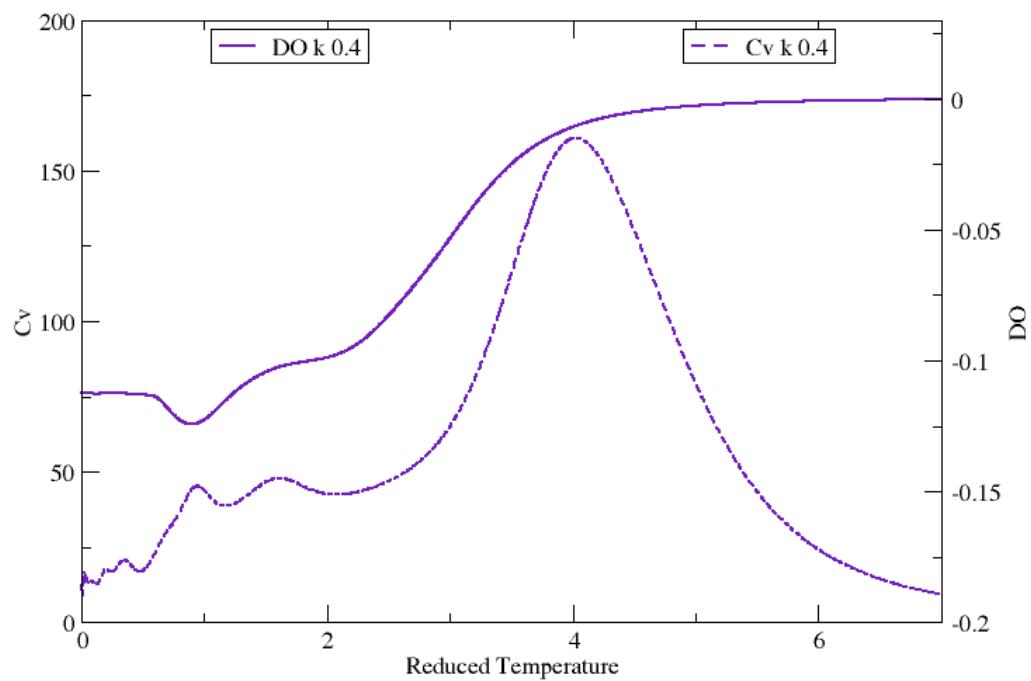
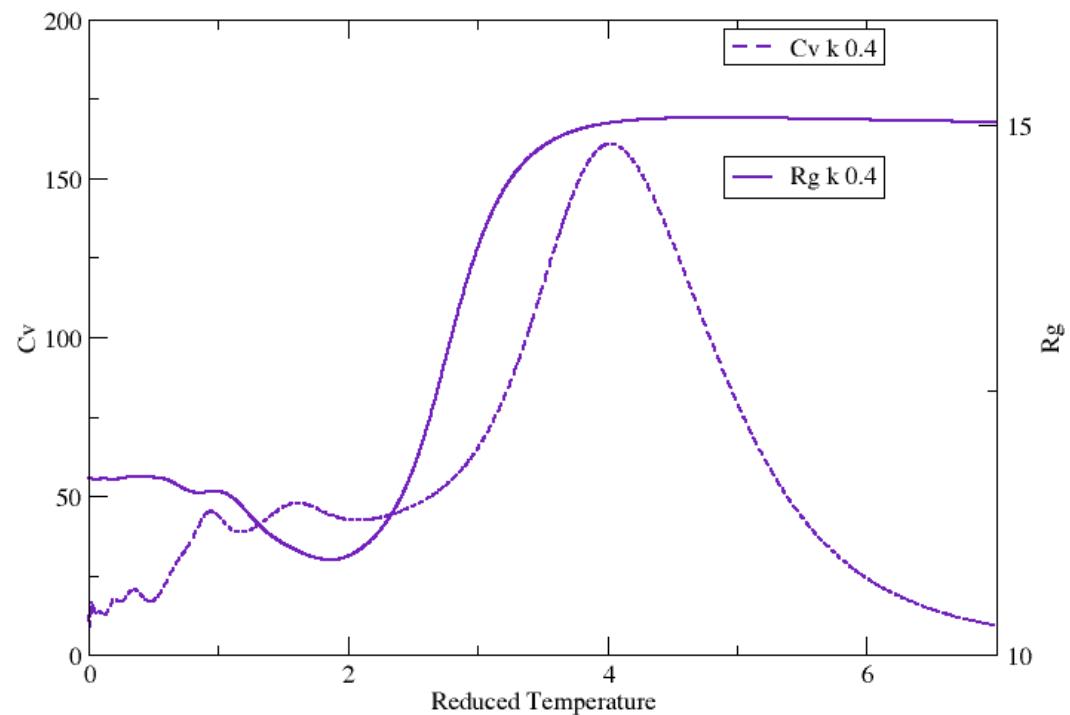
Trial2
 $E=-436.5651$



Trial3
 $E=-441.9837$

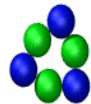


Trial4
 $E=-469.0143$



Kappa 0.41

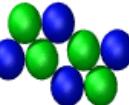
Lowest energy configuration sampled by each trial



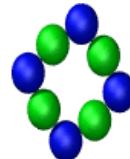
Trial1
 $E=-437.7765$



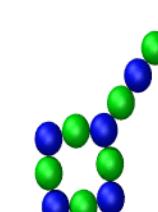
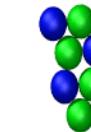
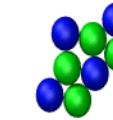
Trial2
 $E=-475.0901$

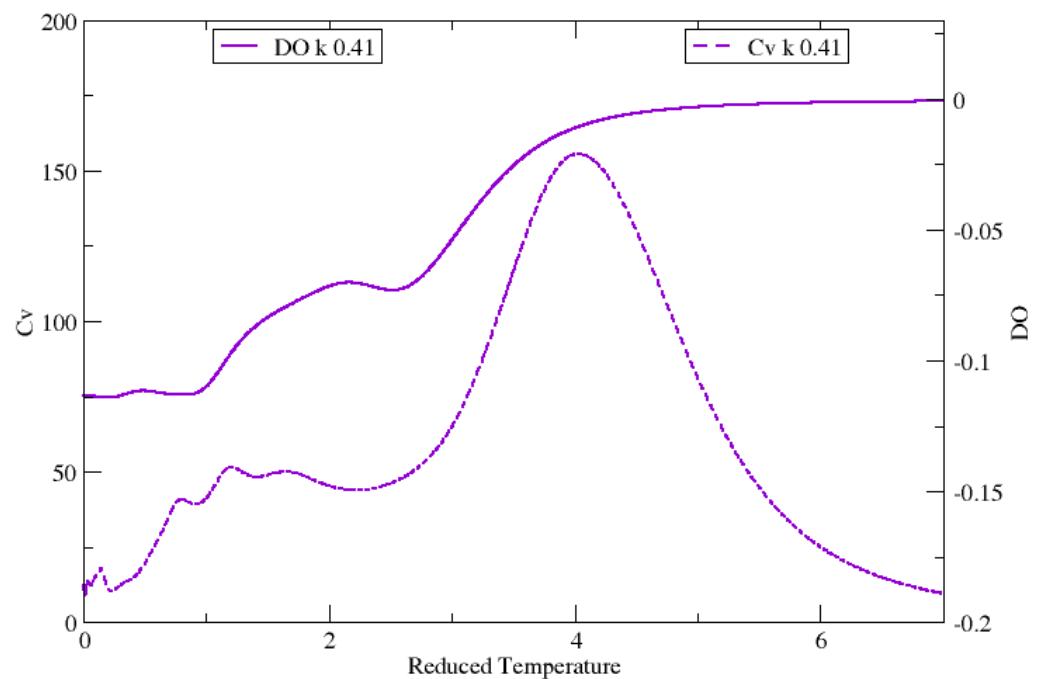
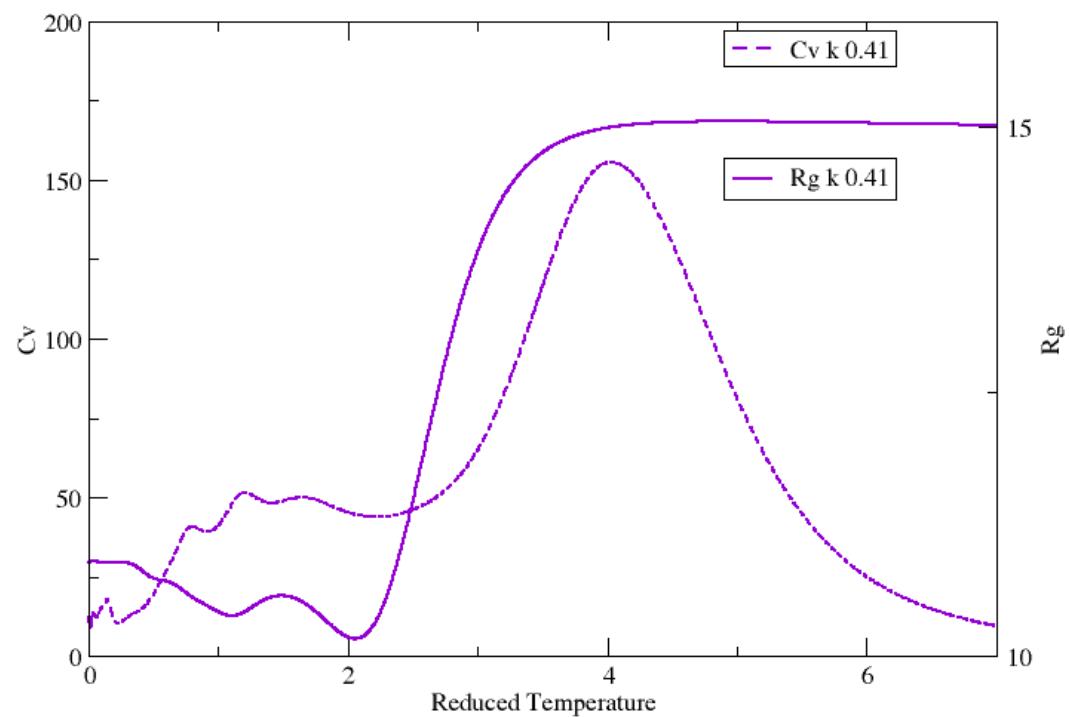


Trial3
 $E=-459.9840$



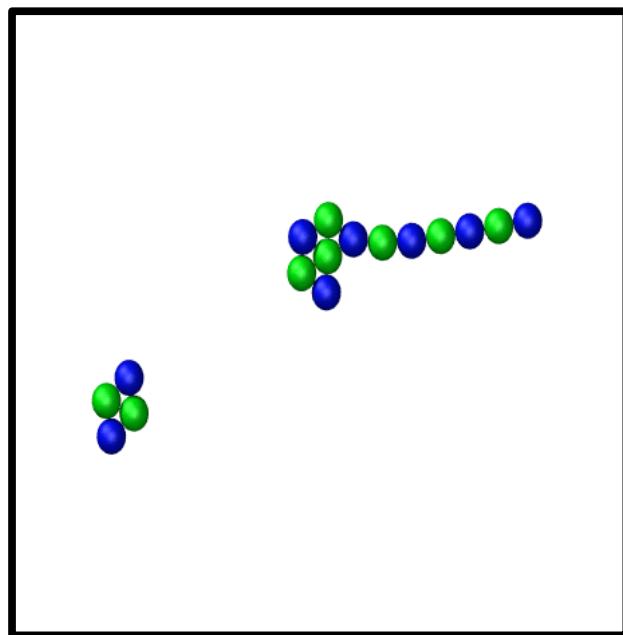
Trial4
 $E=-438.3375$



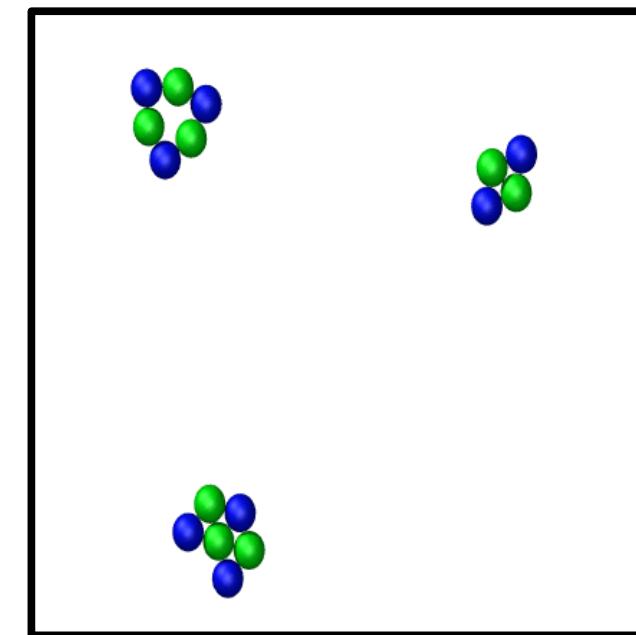


Kappa 0.42

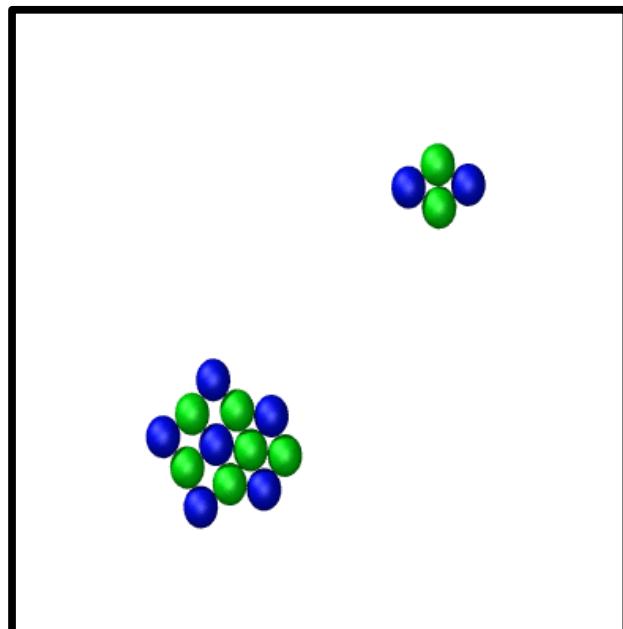
Lowest energy configuration sampled by each trial



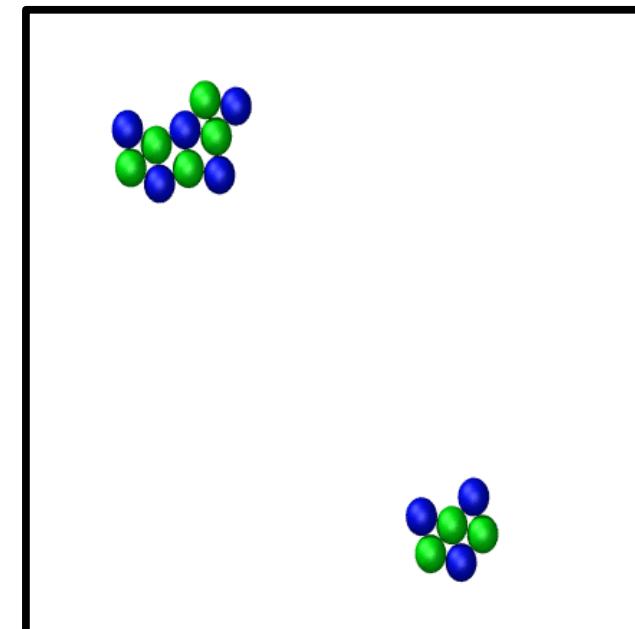
Trial1
 $E=-448.3374$



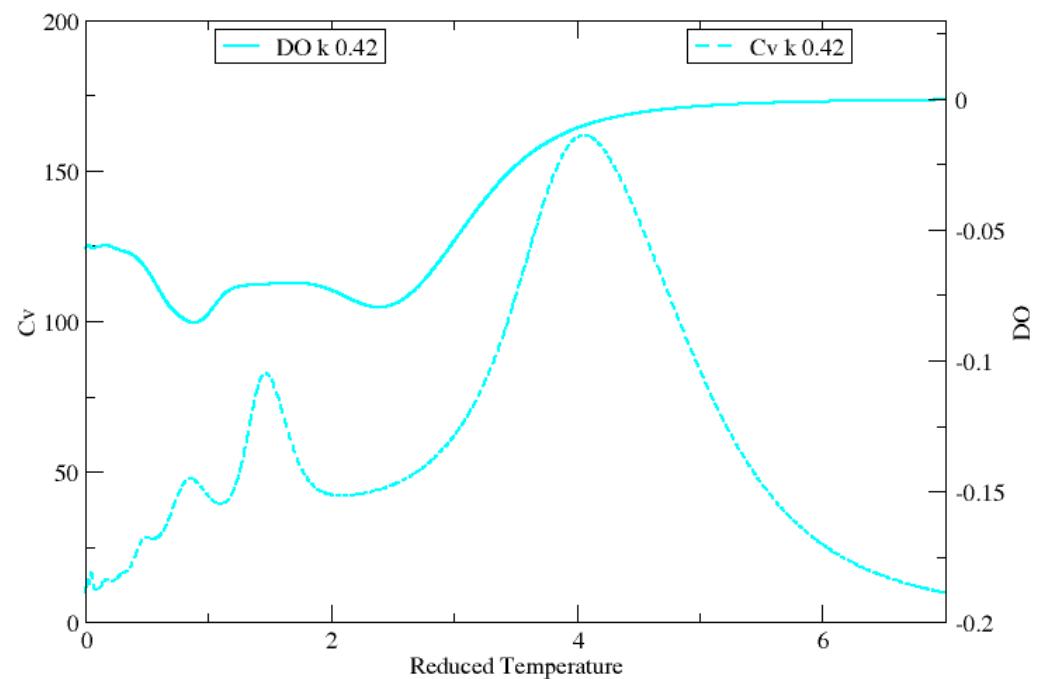
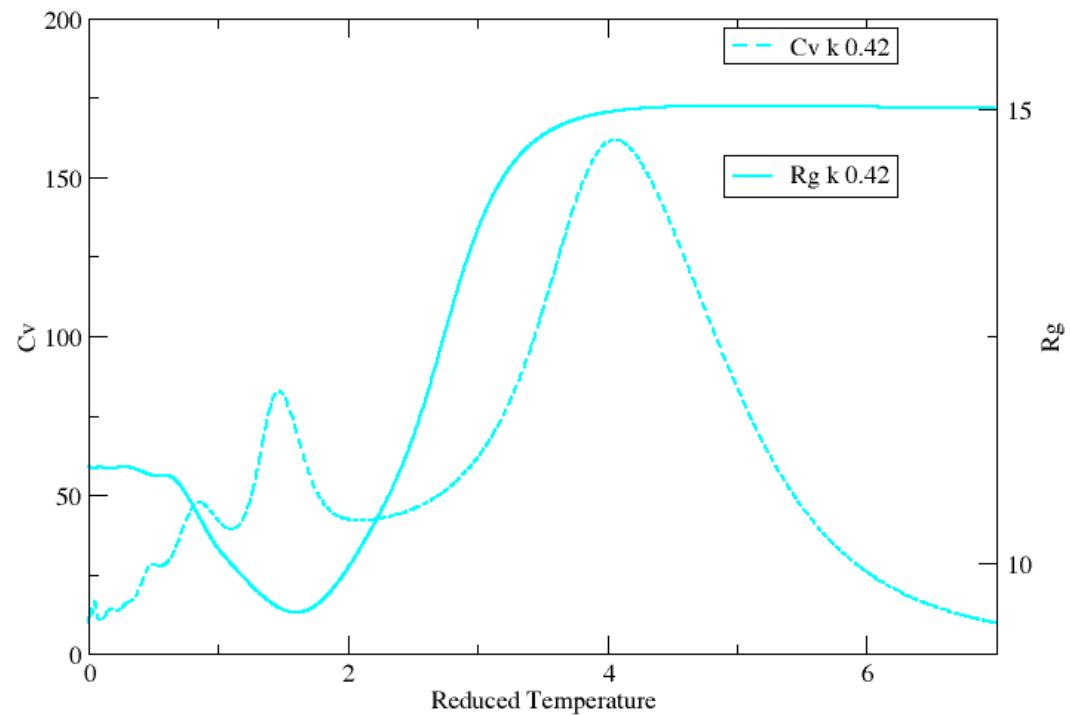
Trial2
 $E=-446.1417$



Trial3
 $E=-489.7814$

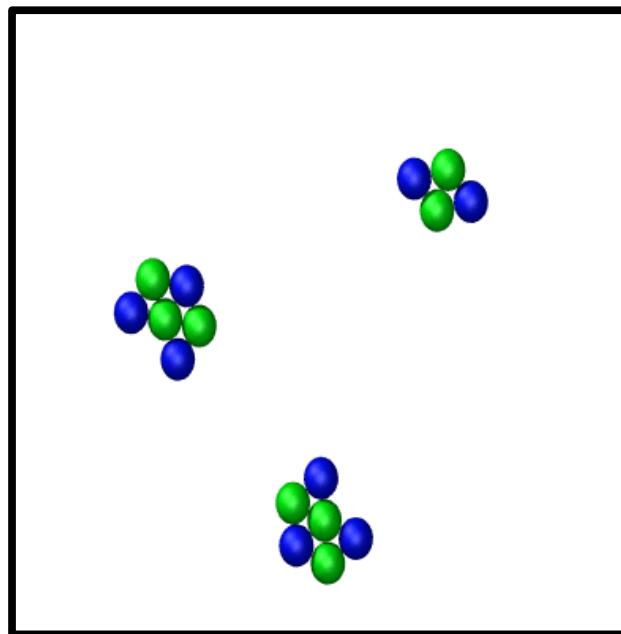


Trial4
 $E=-475.8311$

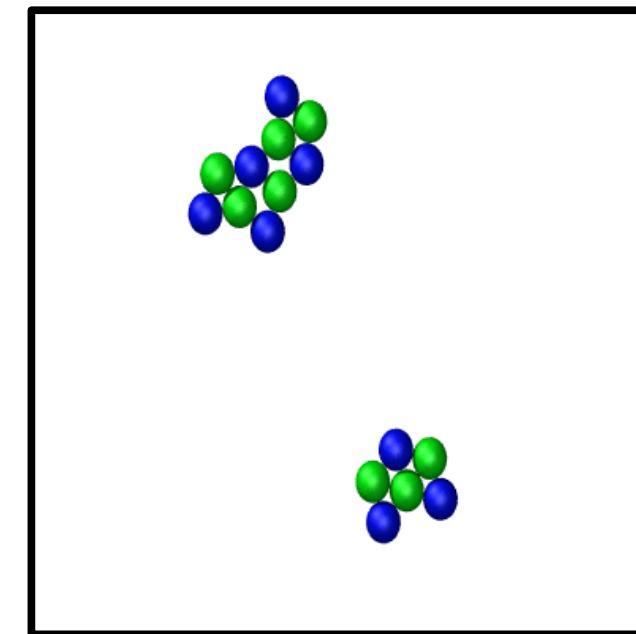


Kappa 0.43

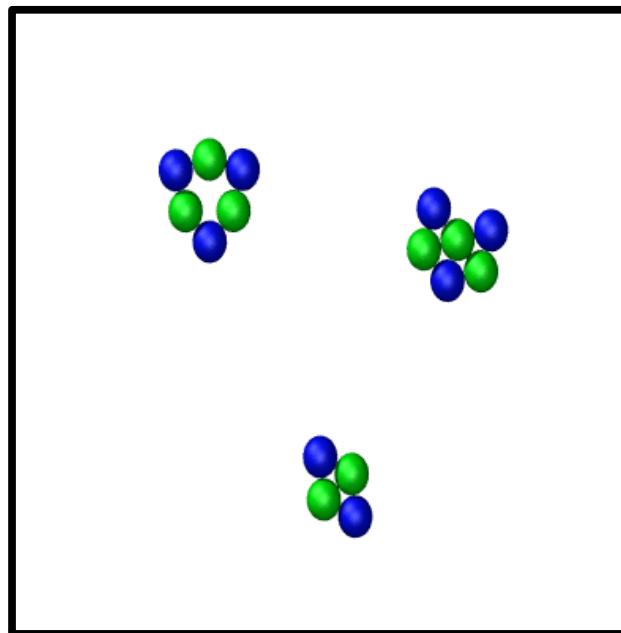
Lowest energy configuration sampled by each trial



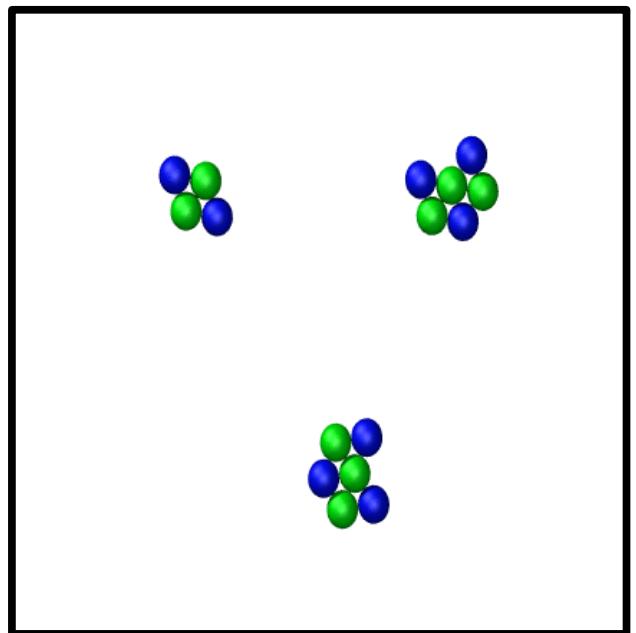
Trial1
 $E=-453.8484$



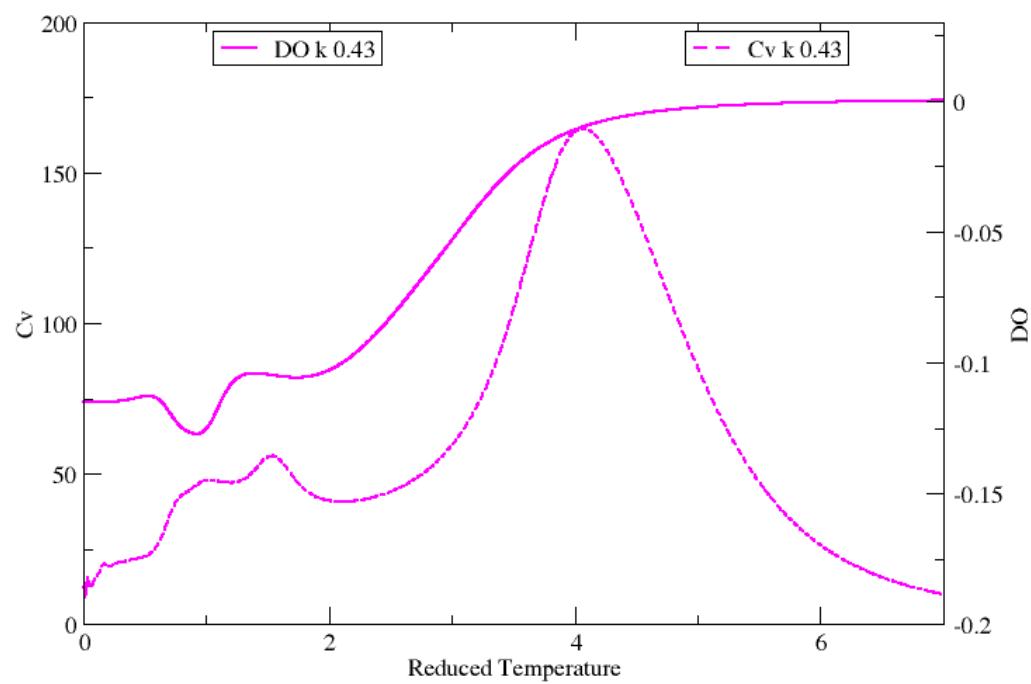
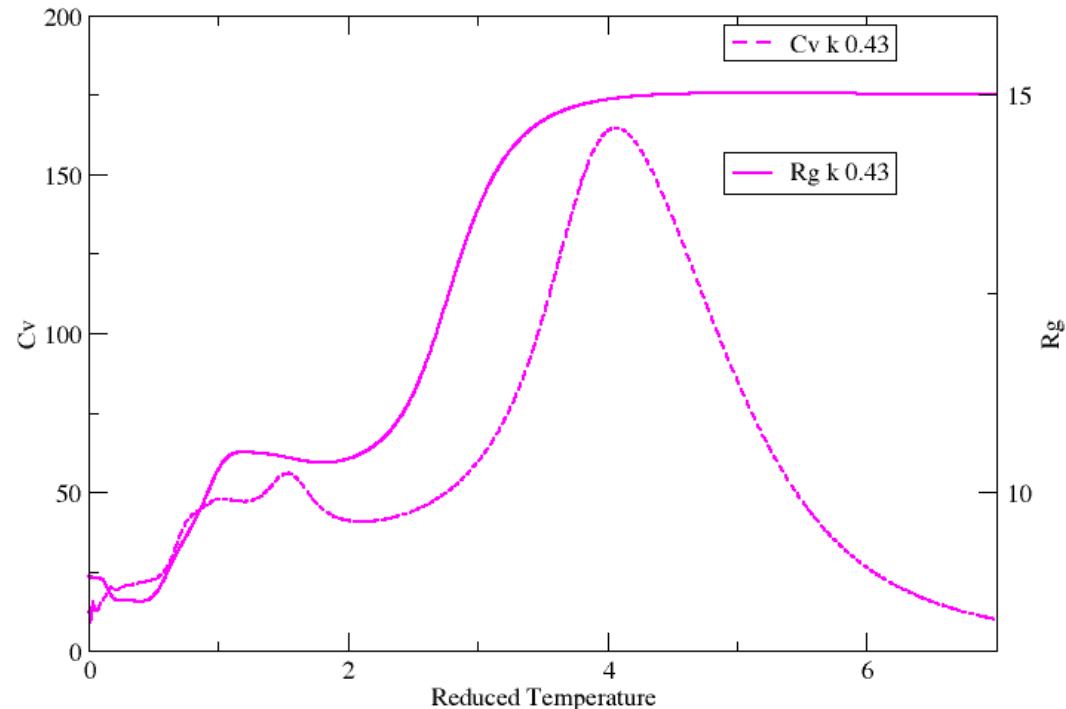
Trial2
 $E=-478.4458$



Trial3
 $E=-446.4729$

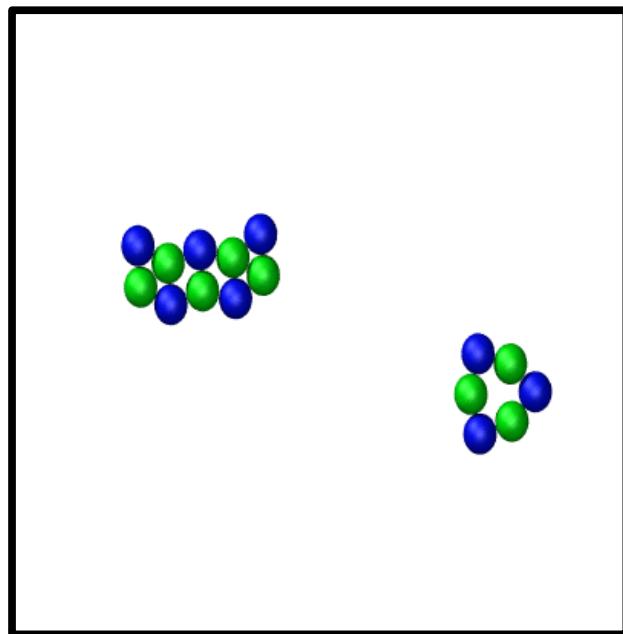


Trial4
 $E=-454.2795$

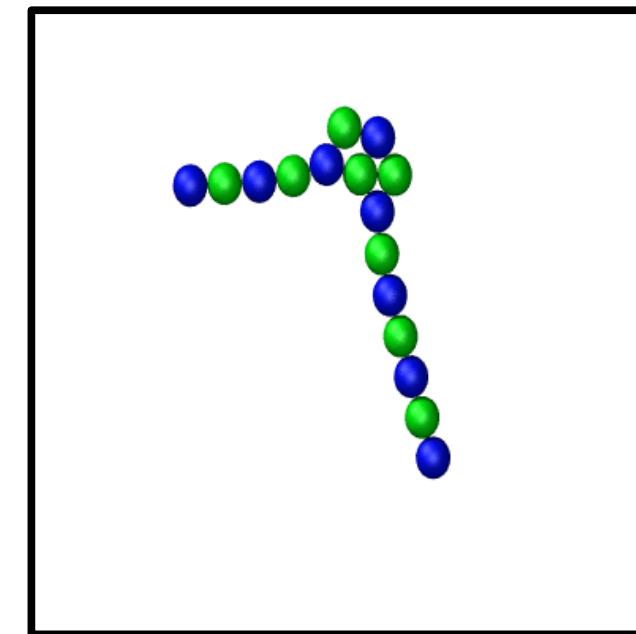


Kappa 0.44

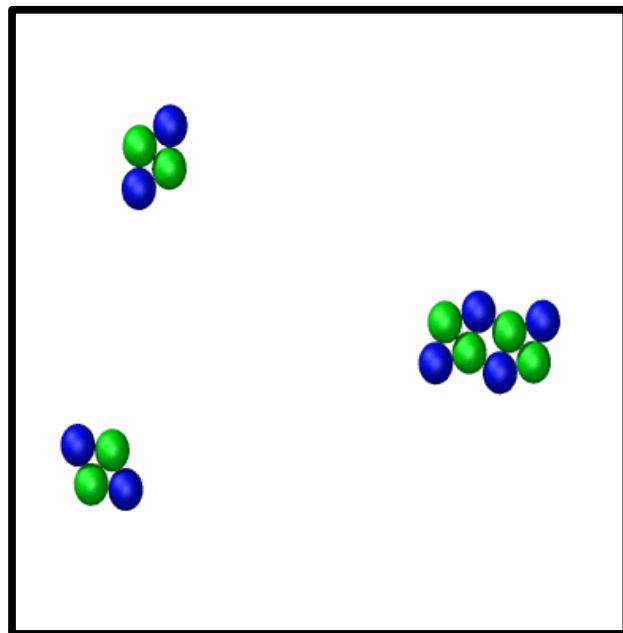
Lowest energy configuration sampled by each trial



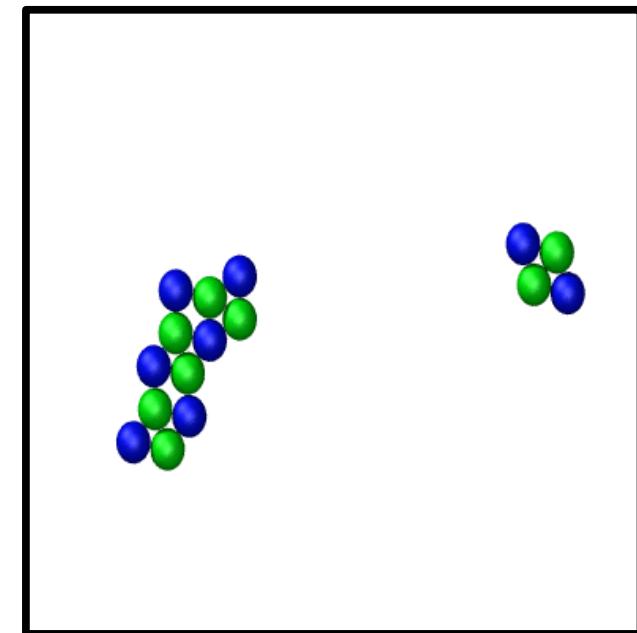
Trial1
 $E=-472.6836$



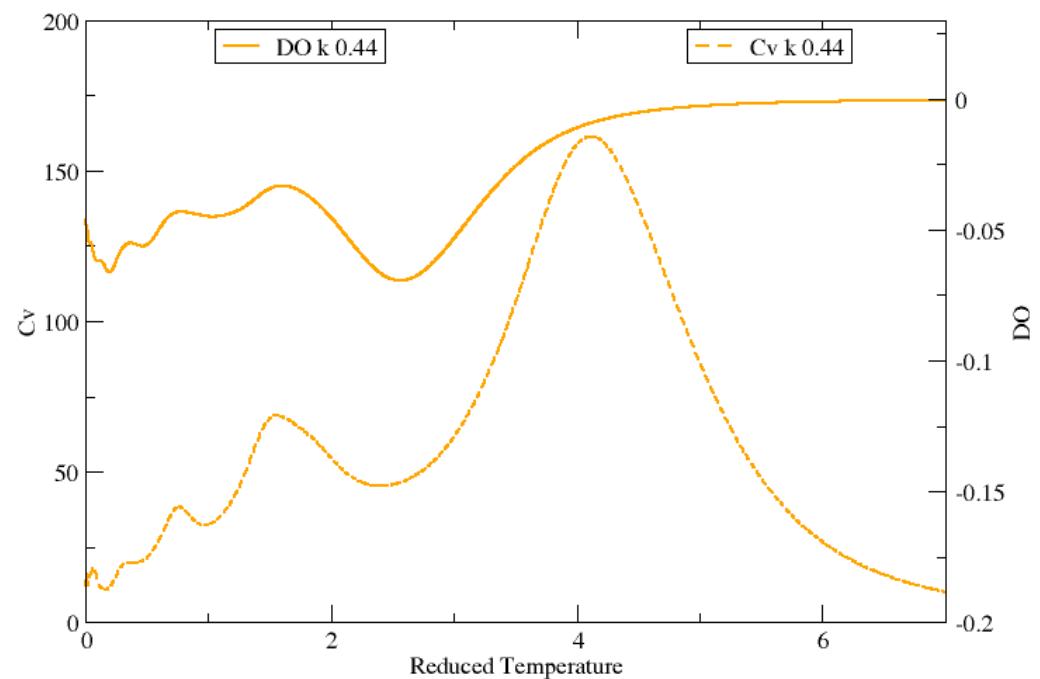
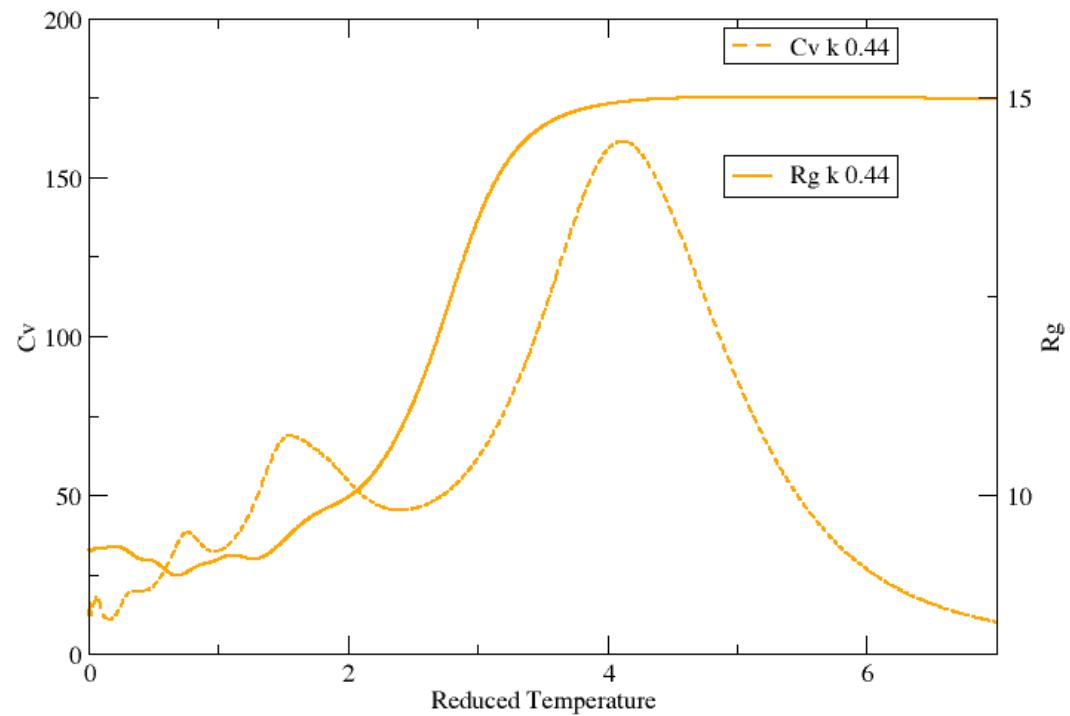
Trial2
 $E=-453.1292$



Trial3
 $E=-459.5056$



Trial4
 $E=-481.4877$

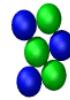


Kappa 0.45

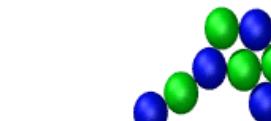
Lowest energy configuration sampled by each trial



Trial1
 $E=-454.8846$



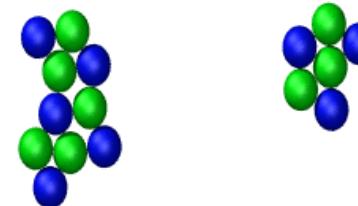
Trial2
 $E=-455.3252$

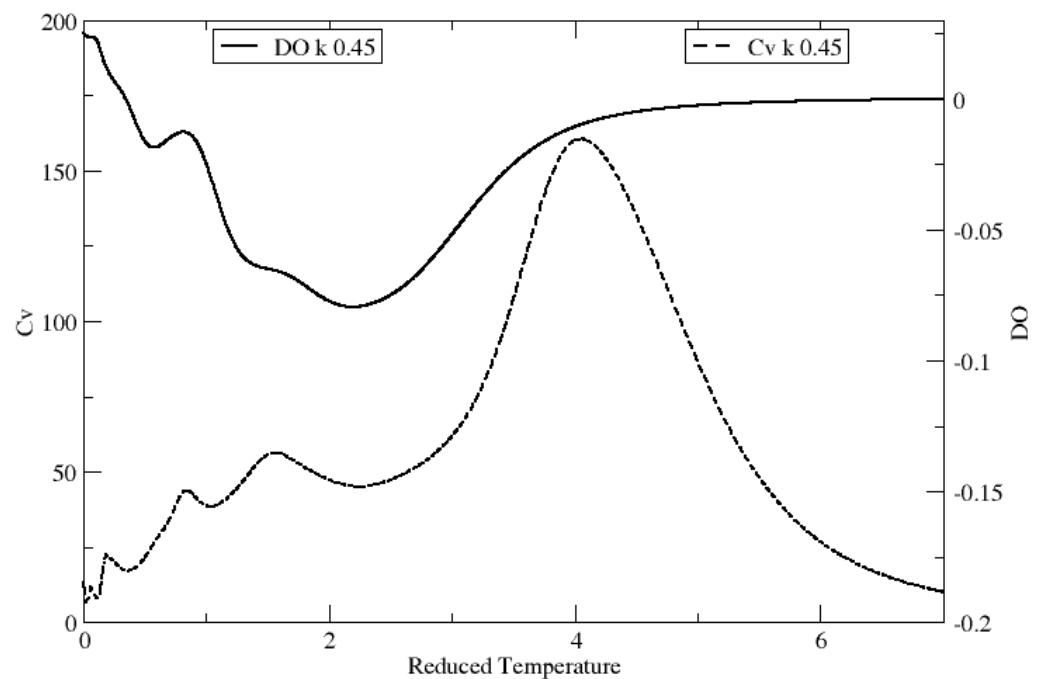
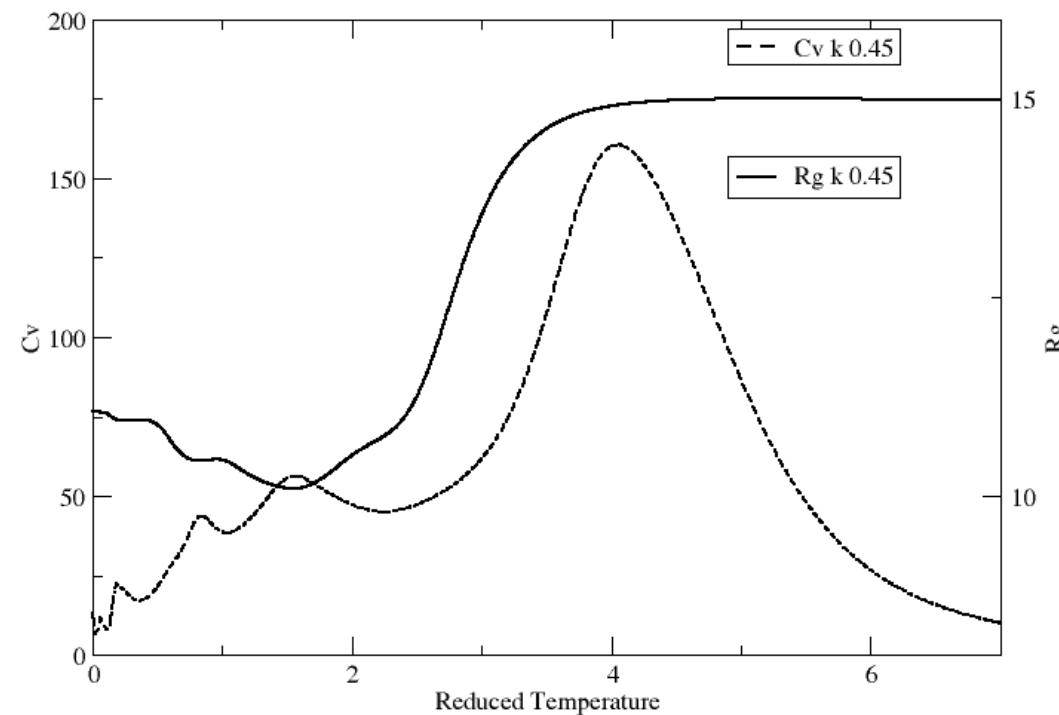


Config sort fail

Trial3
 $E=$

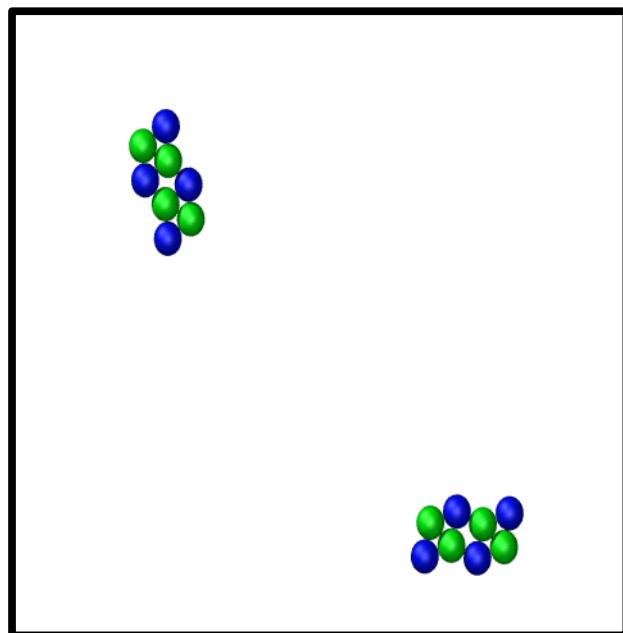
Trial4
 $E=-482.4430$



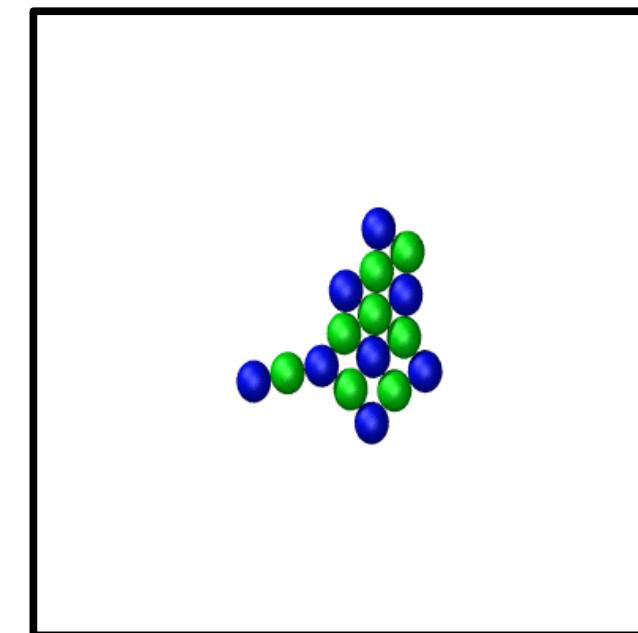


Kappa 0.5

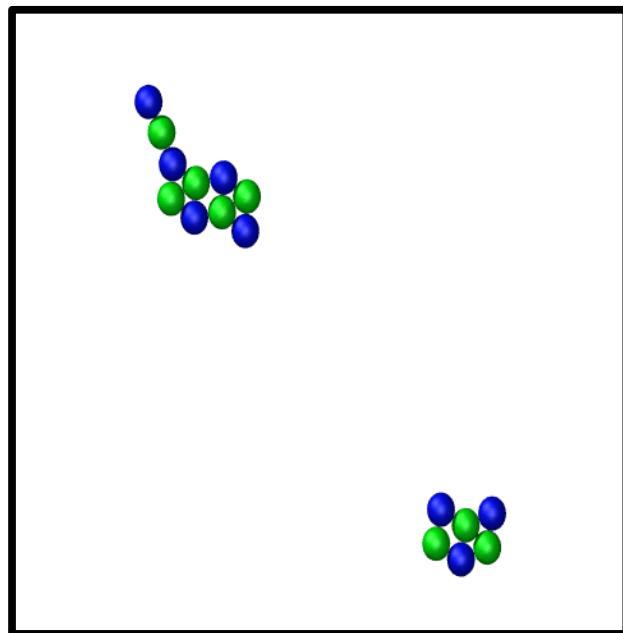
Lowest energy configuration sampled by each trial



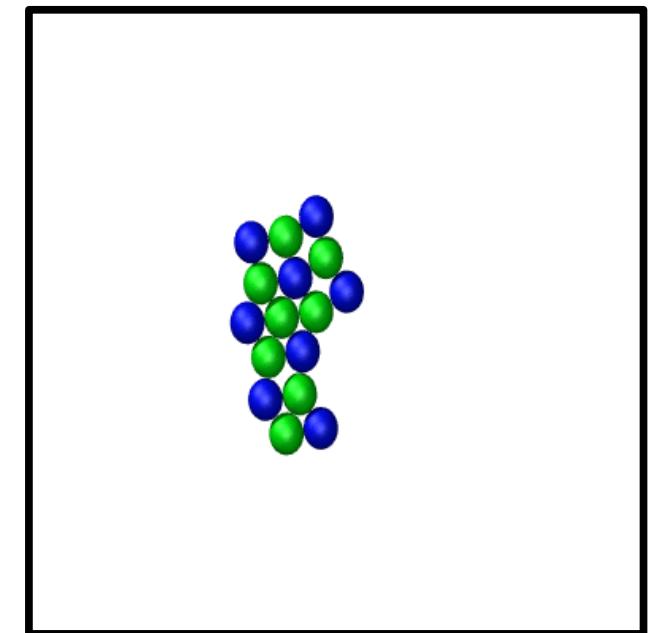
Trial1
 $E=-491.5501$



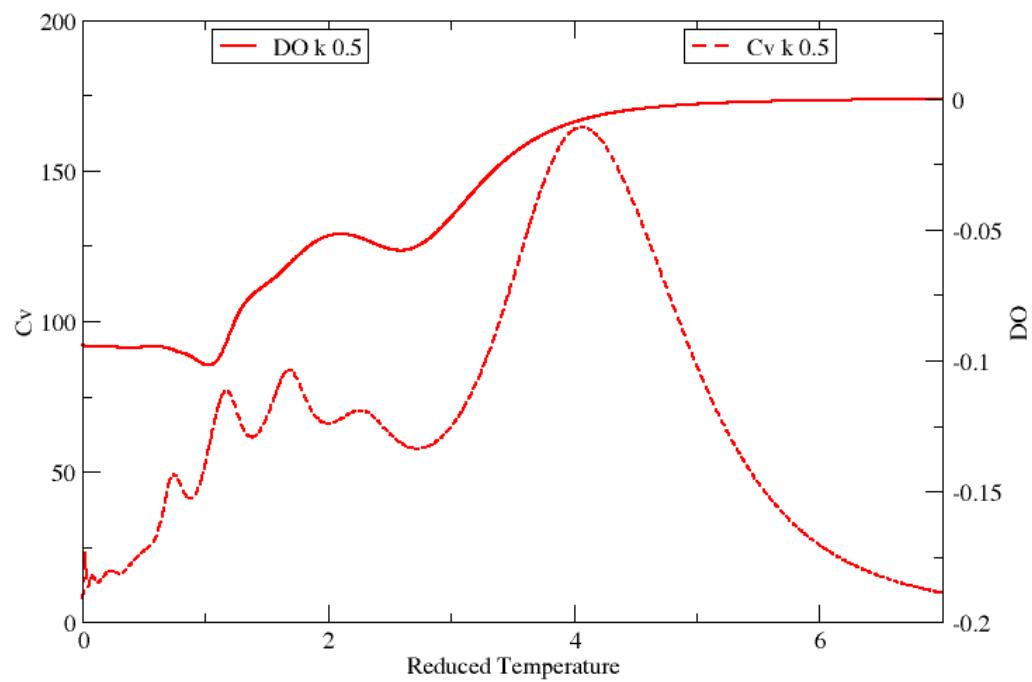
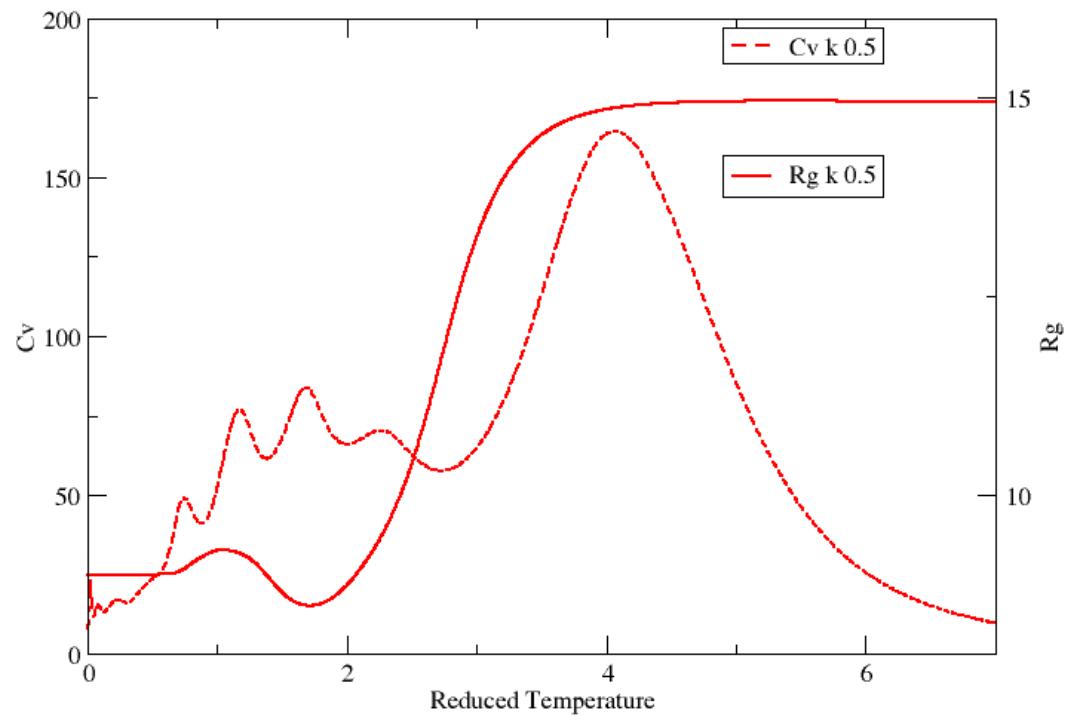
Trial2
 $E=-520.6153$



Trial3
 $E=-474.7168$

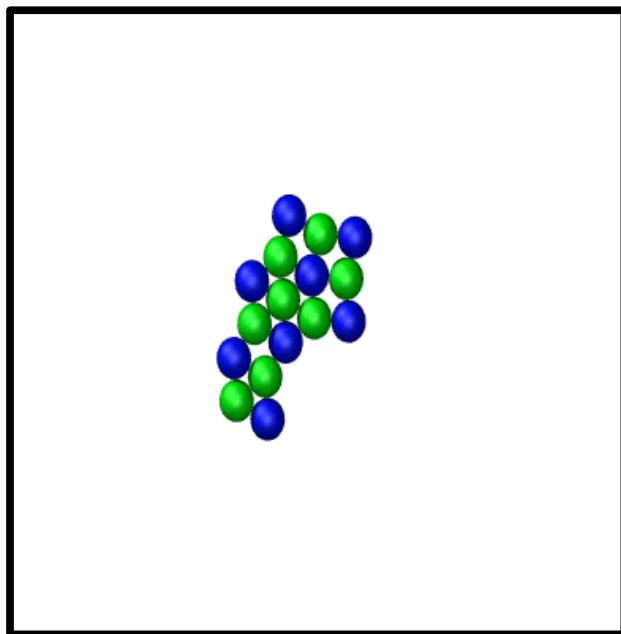


Trial4
 $E=-533.4858$

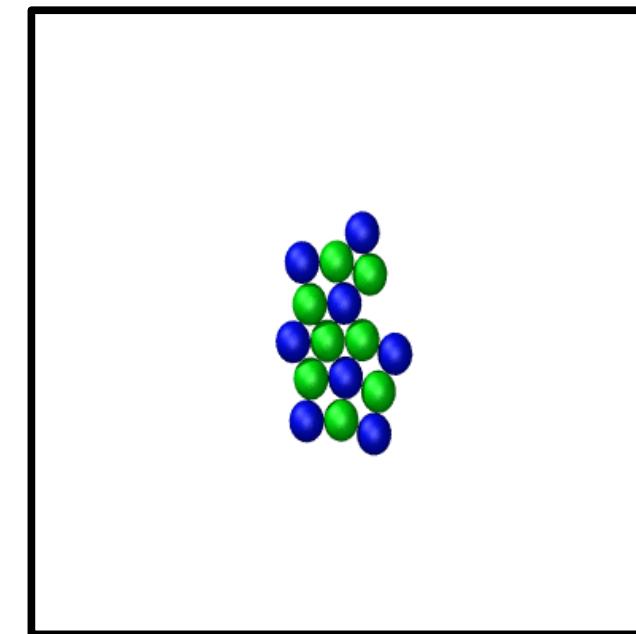


Kappa 0.6

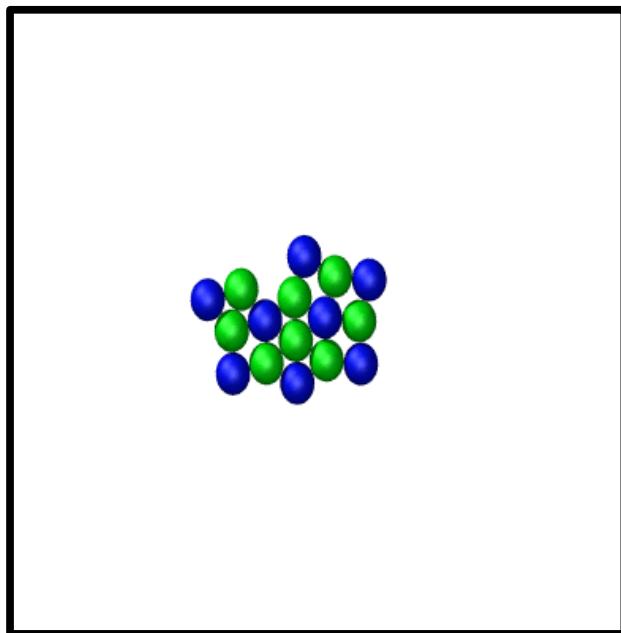
Lowest energy configuration sampled by each trial



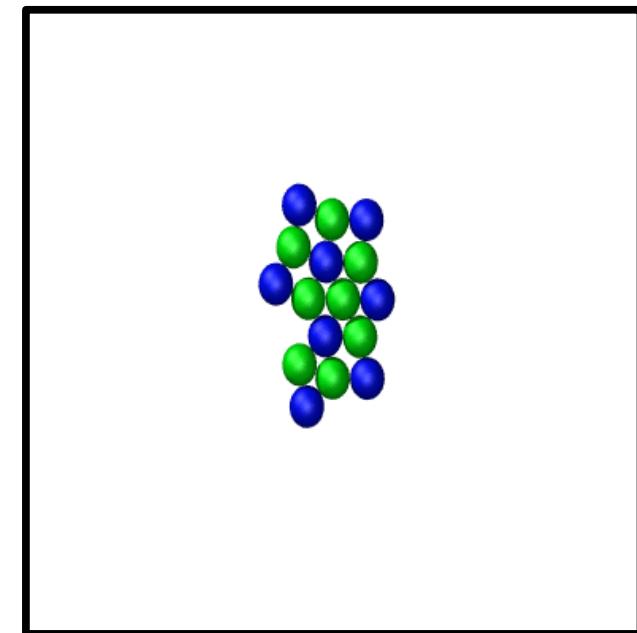
Trial1
 $E=-526.3658$



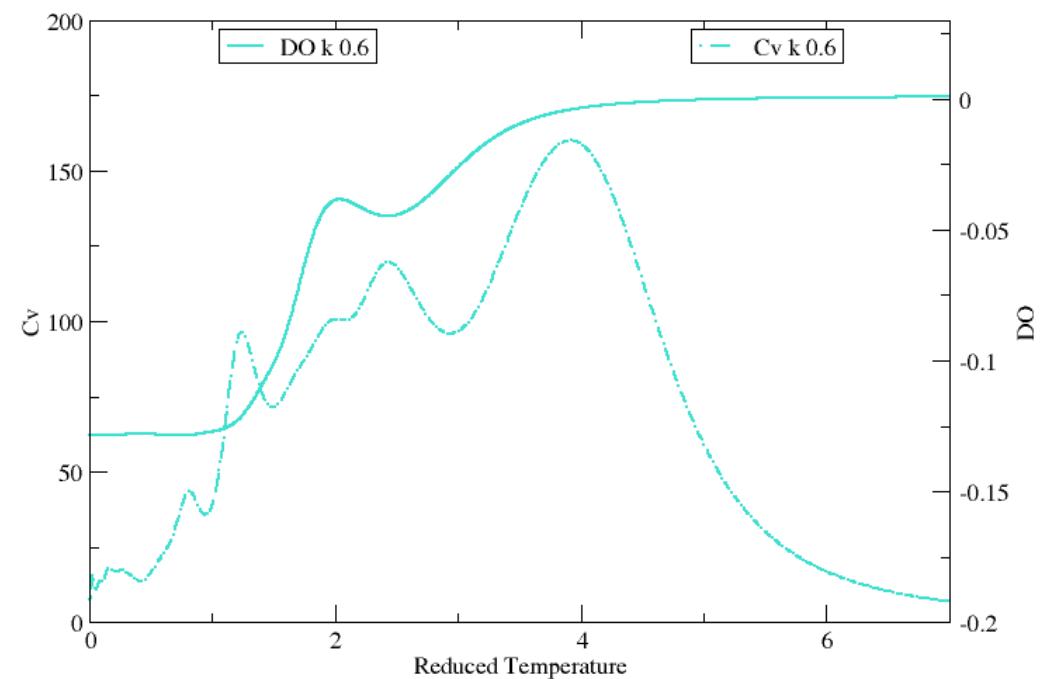
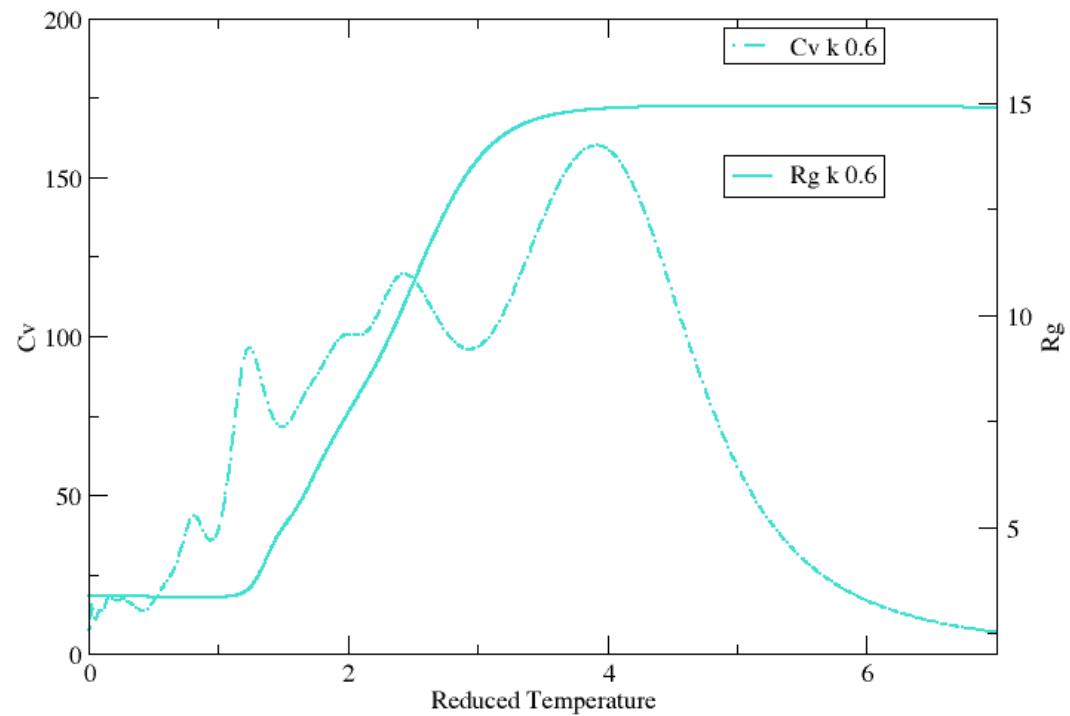
Trial2
 $E=-526.7729$



Trial3
 $E=-526.3855$

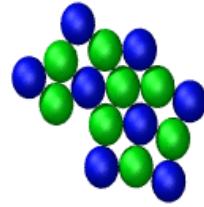


Trial4
 $E=-527.0342$

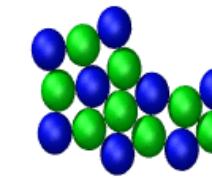


Kappa 0.7

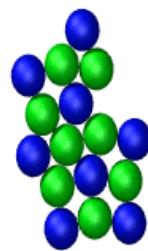
Lowest energy configuration sampled by each trial



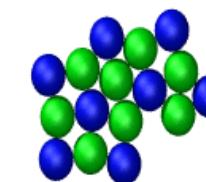
Trial1
 $E=-495.1470$



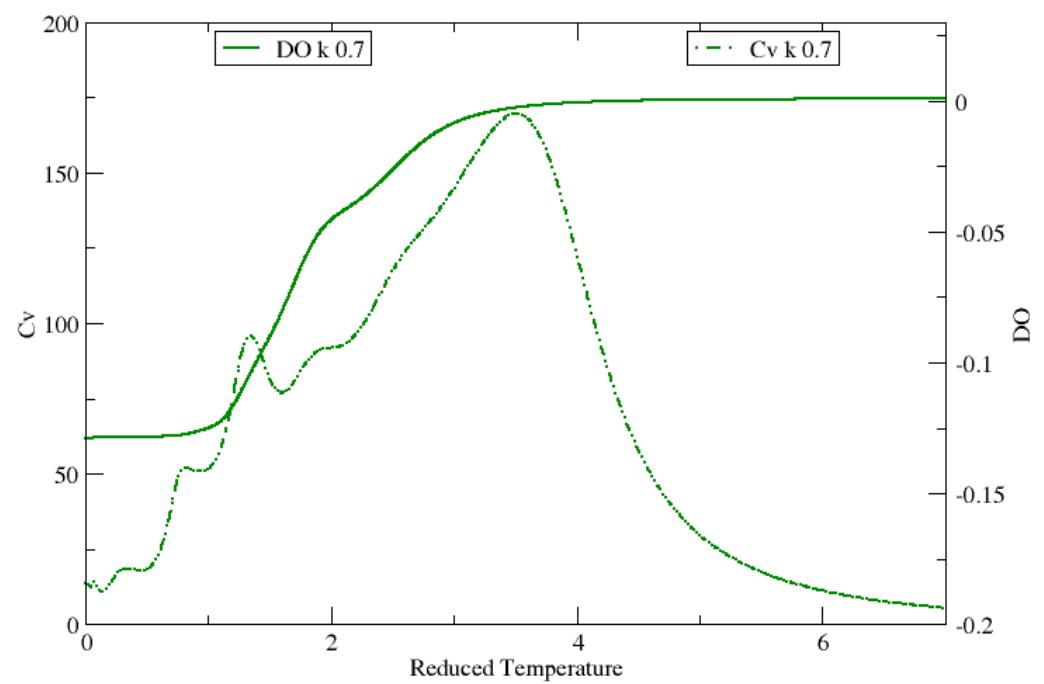
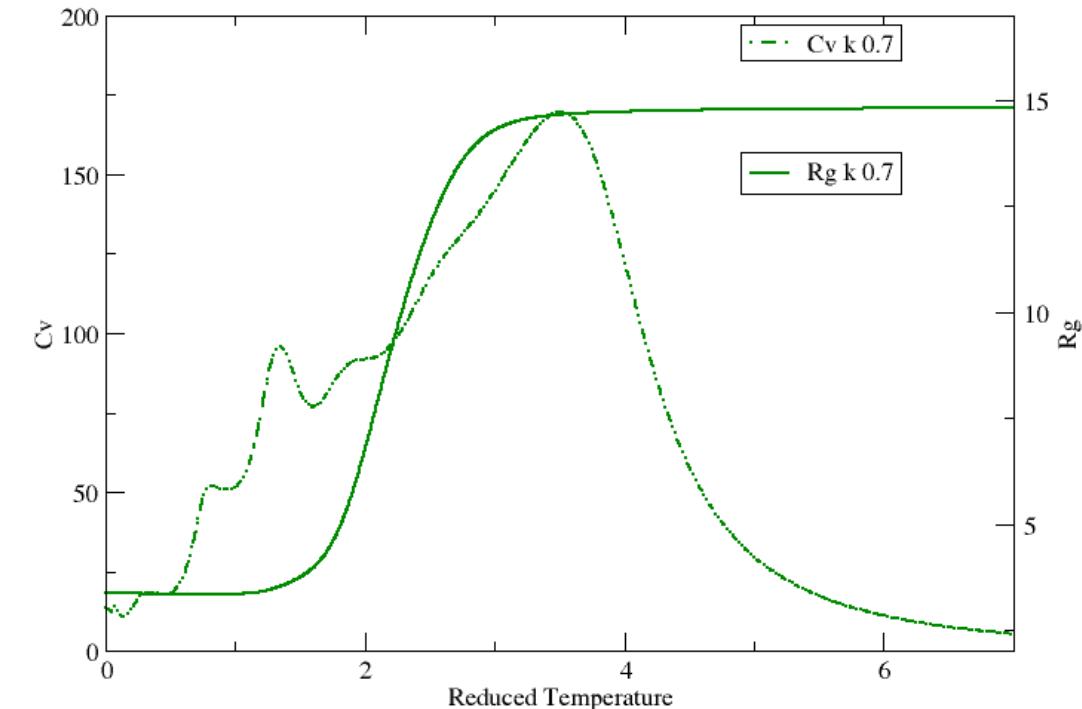
Trial2
 $E=-495.7740$



Trial3
 $E=-495.2534$

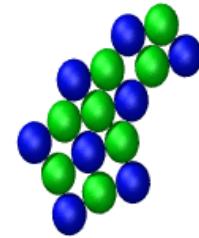


Trial4
 $E=-495.2087$

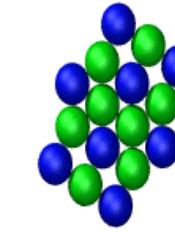


Kappa 0.8

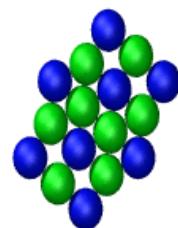
Lowest energy configuration sampled by each trial



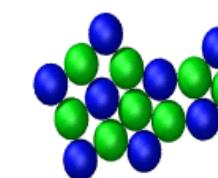
Trial1
 $E=-453.7177$



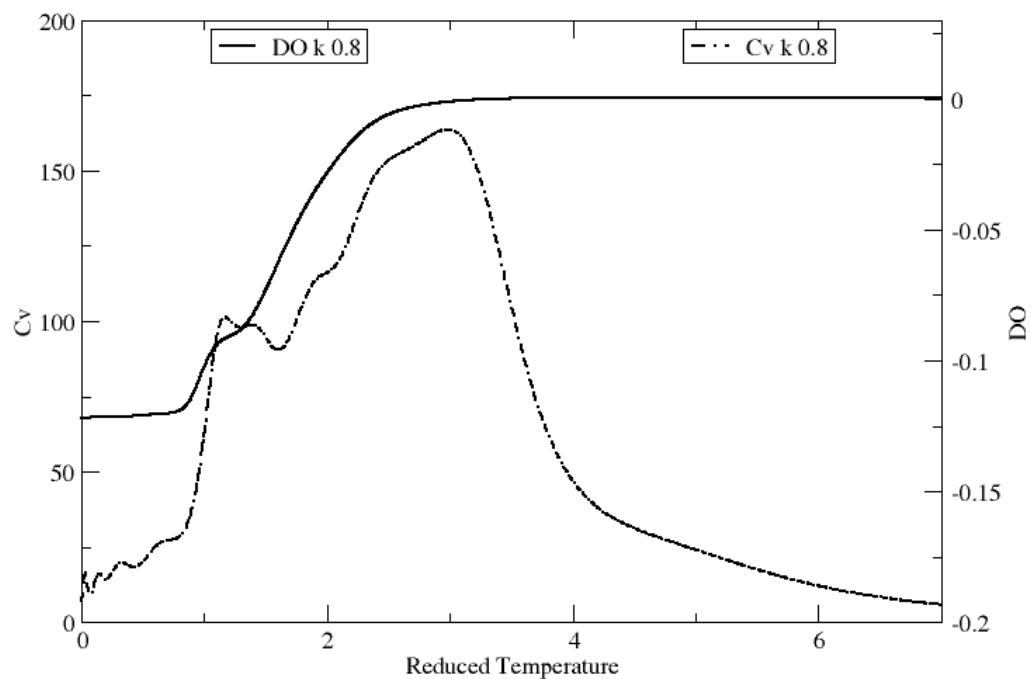
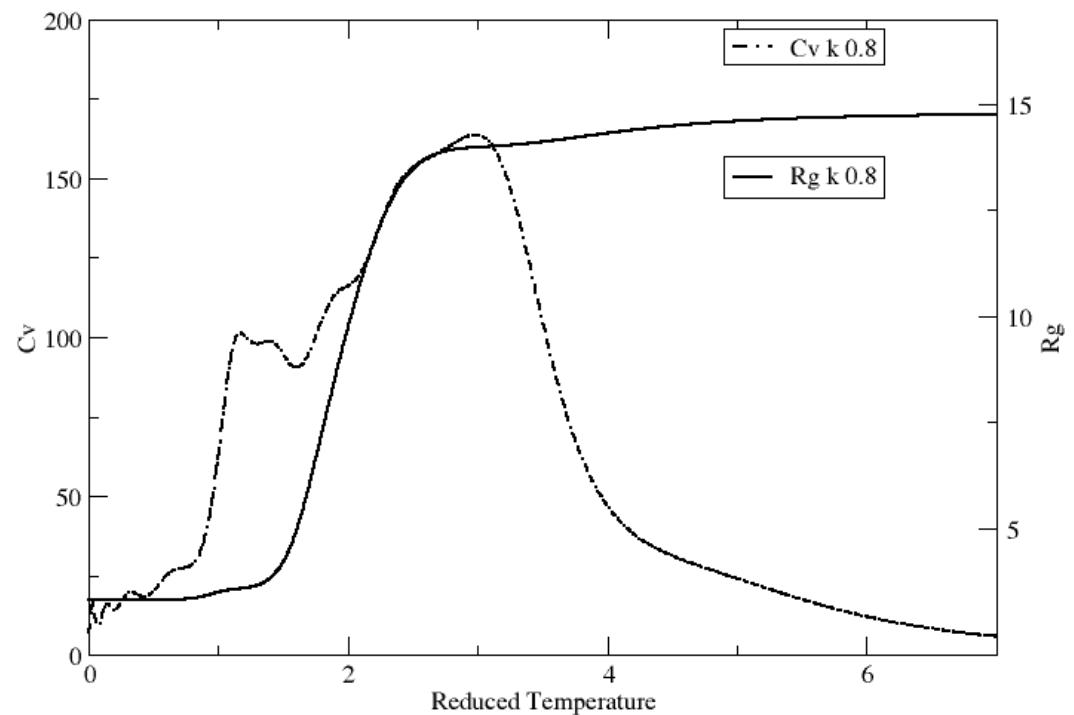
Trial2
 $E=-461.9052$



Trial3
 $E=-461.9688$

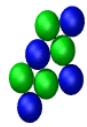


Trial4
 $E=-453.7439$

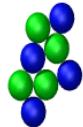


Kappa 0.9

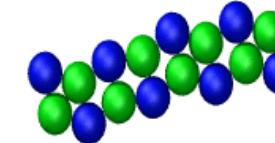
Lowest energy configuration sampled by each trial



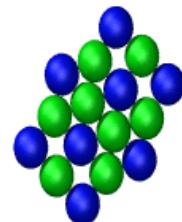
Trial1
 $E=-367.2945$



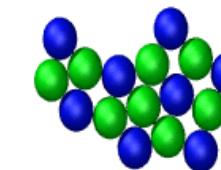
Trial2
 $E=-394.9818$

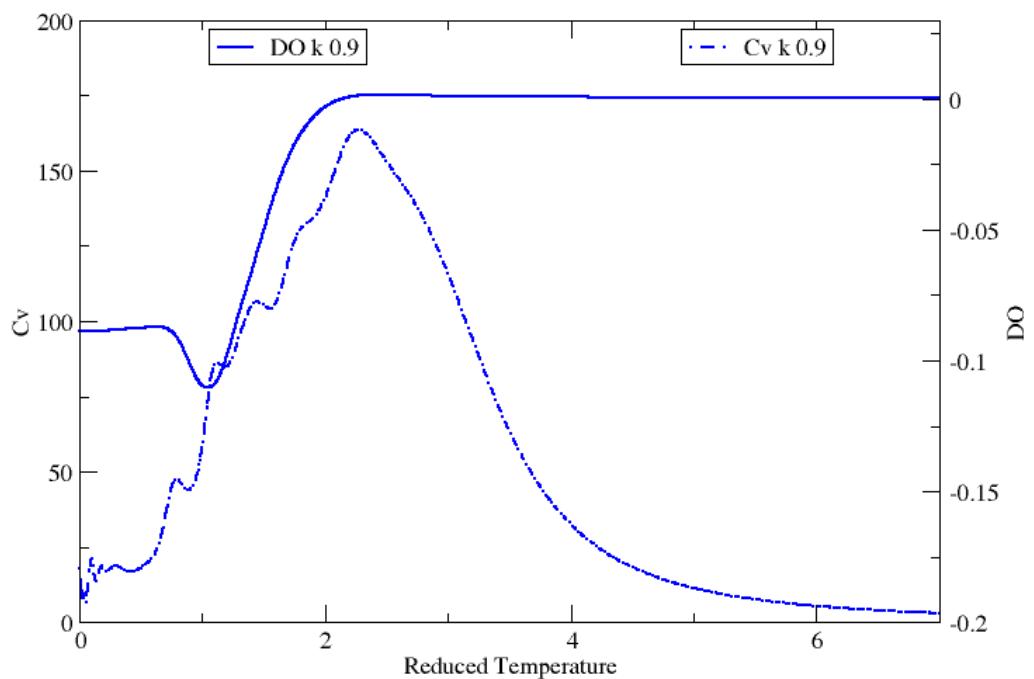
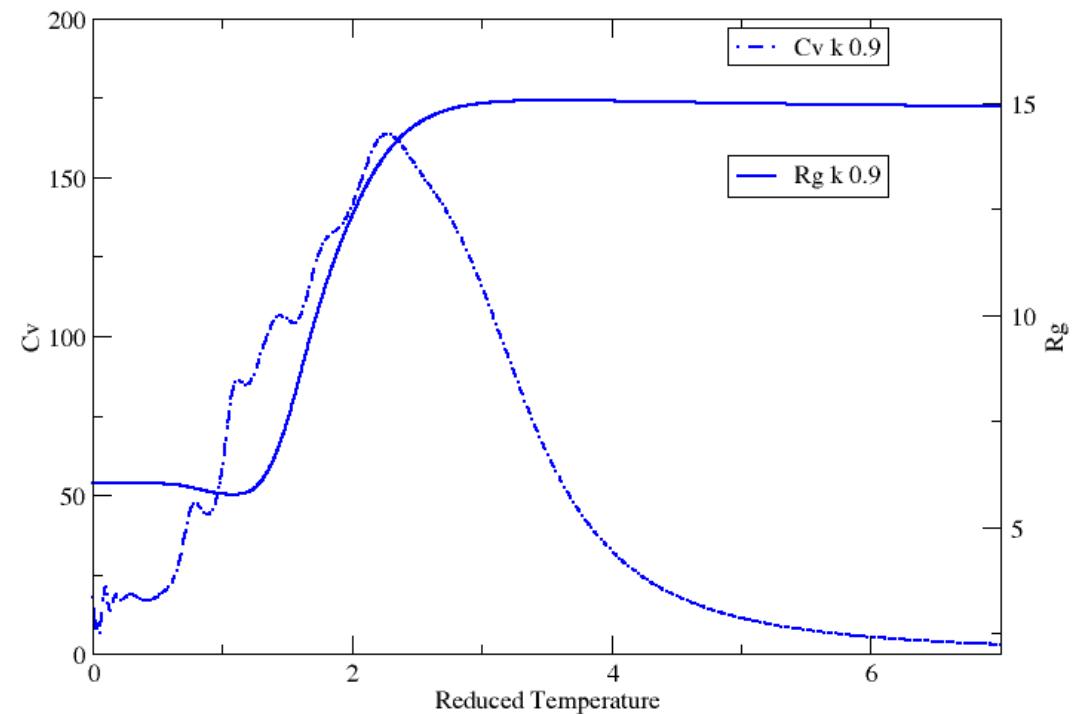


Trial3
 $E=-420.0151$



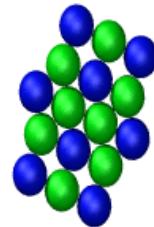
Trial4
 $E=-411.1074$



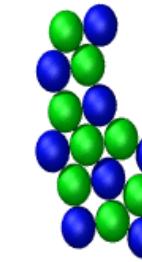


Kappa 1.0

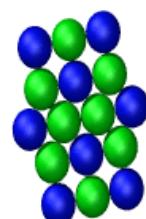
Lowest energy configuration sampled by each trial



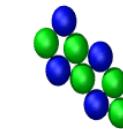
Trial1
 $E=-383.7843$



Trial2
 $E=-375.3606$



Trial3
 $E=-383.9231$



Trial4
 $E=-334.0664$

