Results of relaxation with different parameters

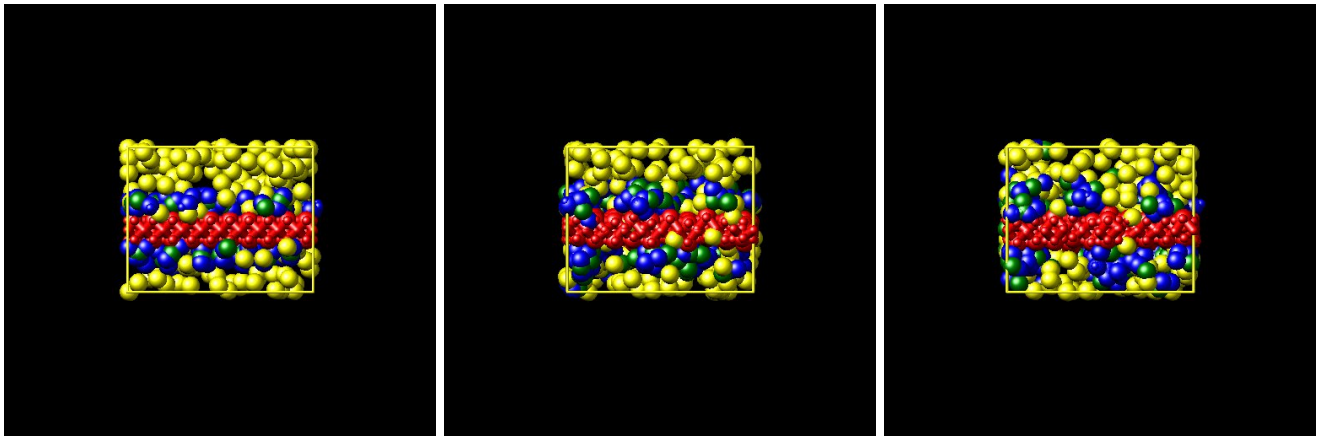
September 17, 2019

One

One-one

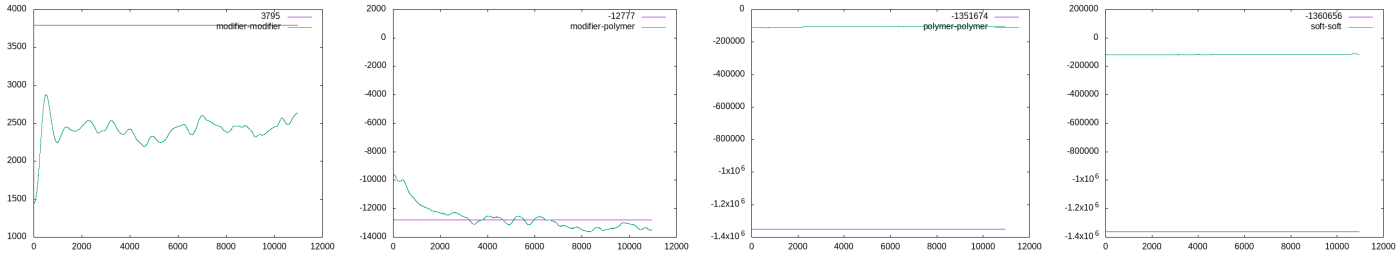
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.001
pair_coeff 3 4 lj/cut/soft 0.05275 10 3 3
pair_coeff 4 4 lj/cut/soft 0.09150 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=50, r=0.8	a=50, r=0.8	a=150, r=0.8
		a=50, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 1



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

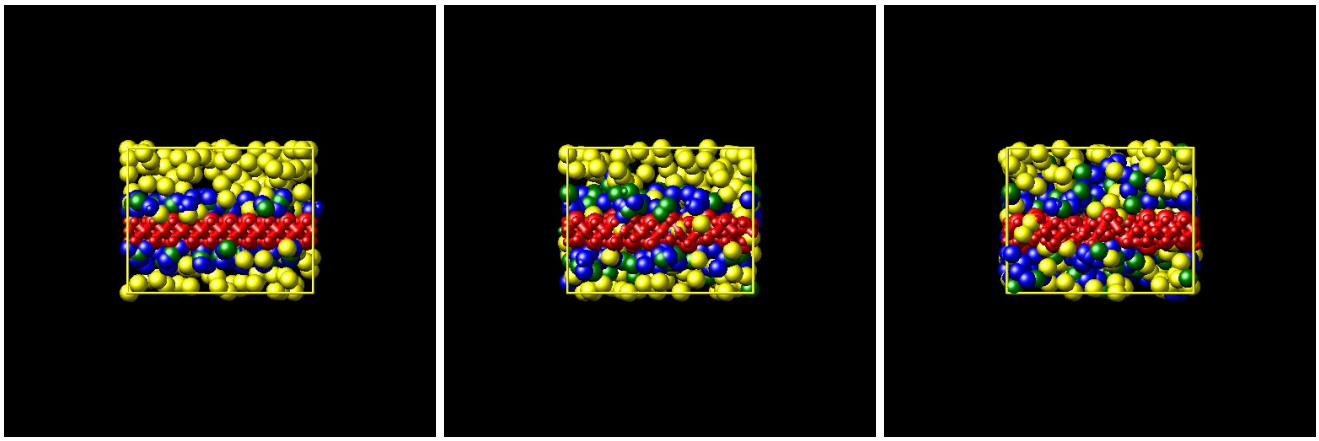
Figure 2

Increase mod-mod repulsion
Increase poly-poly attraction

One-two

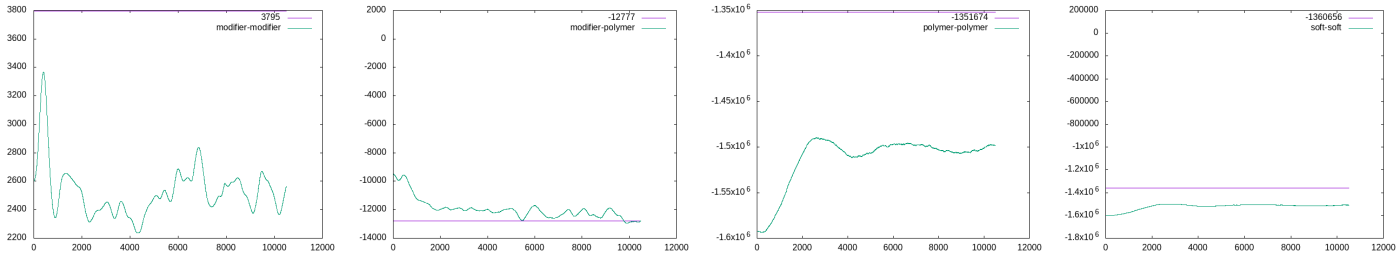
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.001
pair_coeff 3 4 lj/cut/soft 0.05275 10 3 3
pair_coeff 4 4 lj/cut/soft 1 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=100, r=0.8	a=100, r=0.8	a=150, r=0.8
		a=50, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 3



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

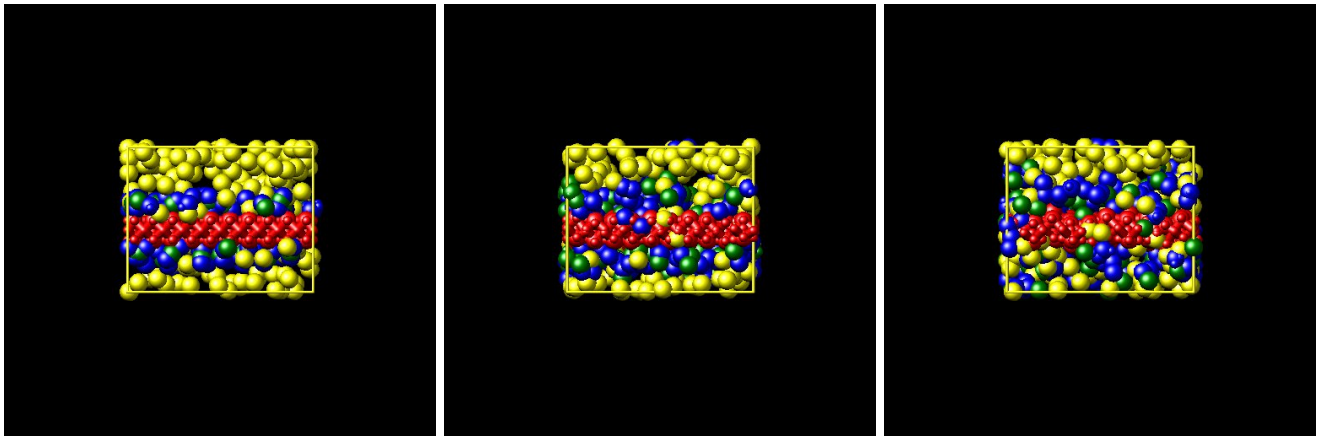
Figure 4

Increase mod-mod repulsion
Slightly decrease poly-poly attraction

One-three

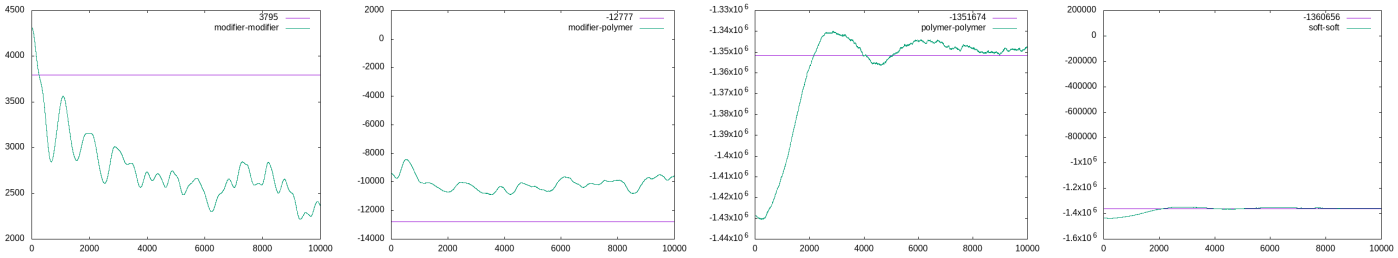
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.001
pair_coeff 3 4 lj/cut/soft 0.05275 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=100, r=0.8	a=150, r=0.8	a=150, r=0.8
		a=150, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 5



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

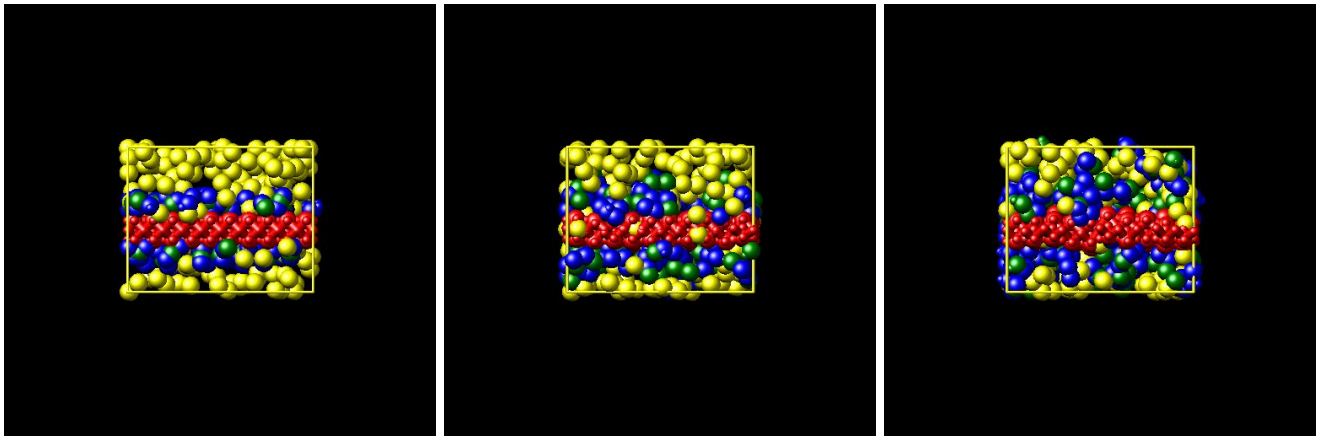
Figure 6

Slightly increase mod-mod repulsion
Slightly increase mod-poly attraction

One-four

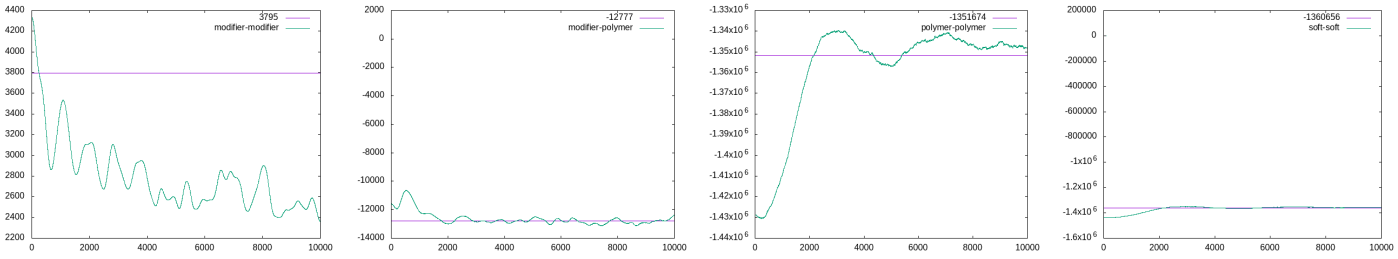
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.001
pair_coeff 3 4 lj/cut/soft 0.06 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=150, r=0.8	a=150, r=0.8	a=150, r=0.8
		a=150, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 7



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

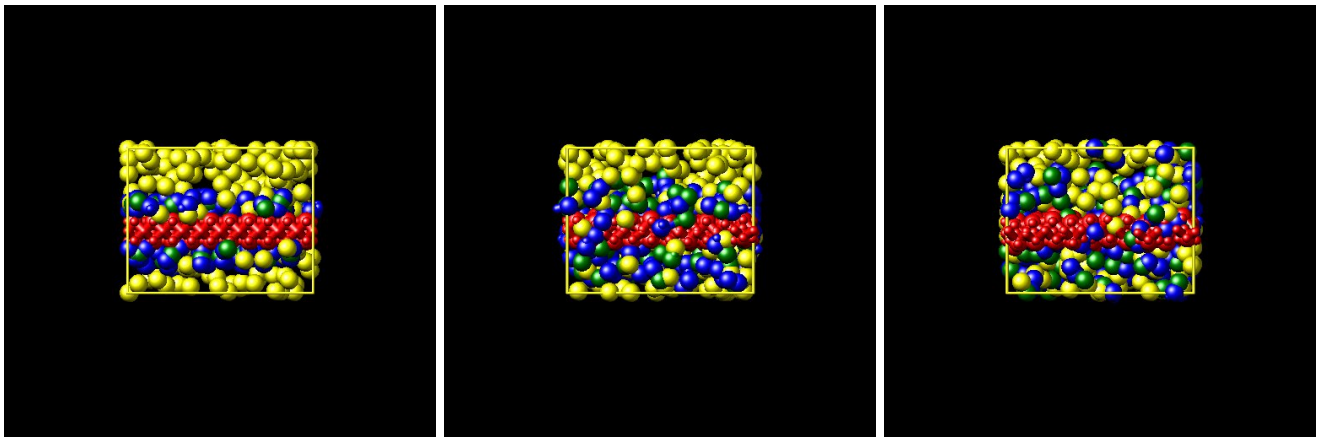
Figure 8

Increase mod-mod repulsion

One-five

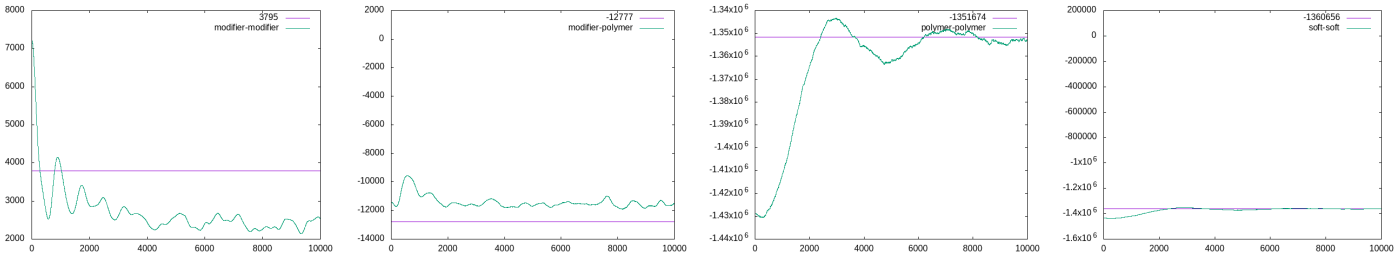
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.001
pair_coeff 3 4 lj/cut/soft 0.06 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=250, r=0.8	a=250, r=0.8	a=150, r=0.8
		a=250, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 9



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

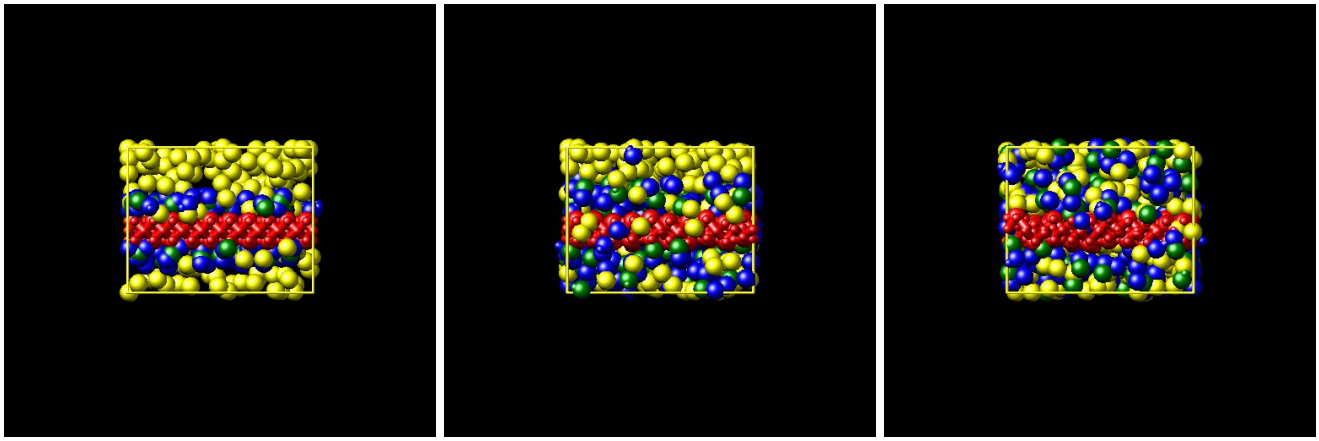
Figure 10

Sloghtly increase mod-mod repulsion
Sloghtly increase mod-poly repulsion

One-six

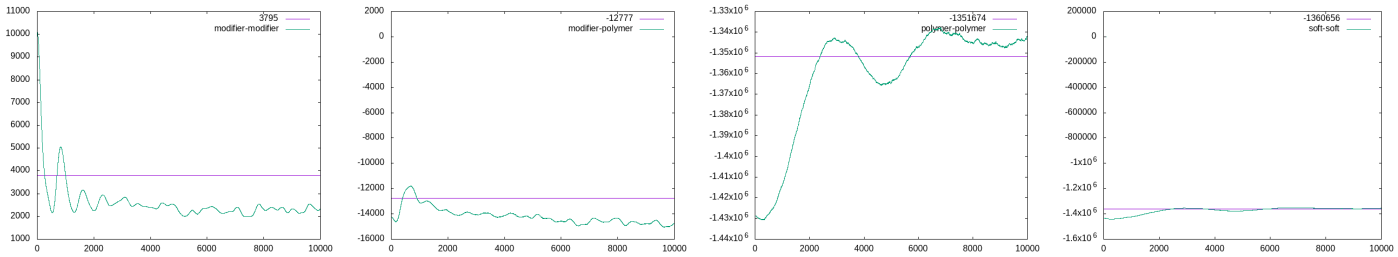
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.001
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=350, r=0.8	a=350, r=0.8	a=150, r=0.8
		a=350, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 11



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

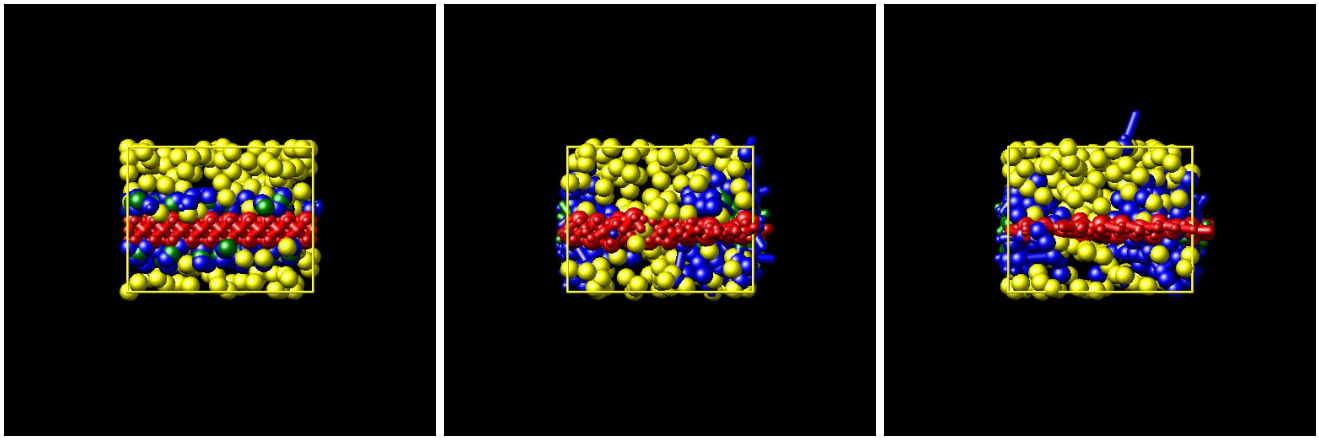
Figure 12

Sloghtly increase mod-mod repulsion
Sloghtly increase mod-poly repulsion

One-seven

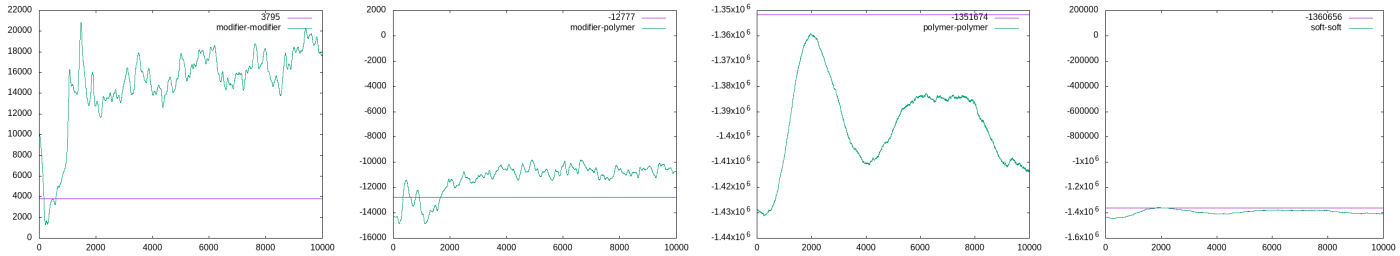
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.1
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=350, r=0.8	a=350, r=0.8	a=150, r=0.8
		a=350, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 13



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

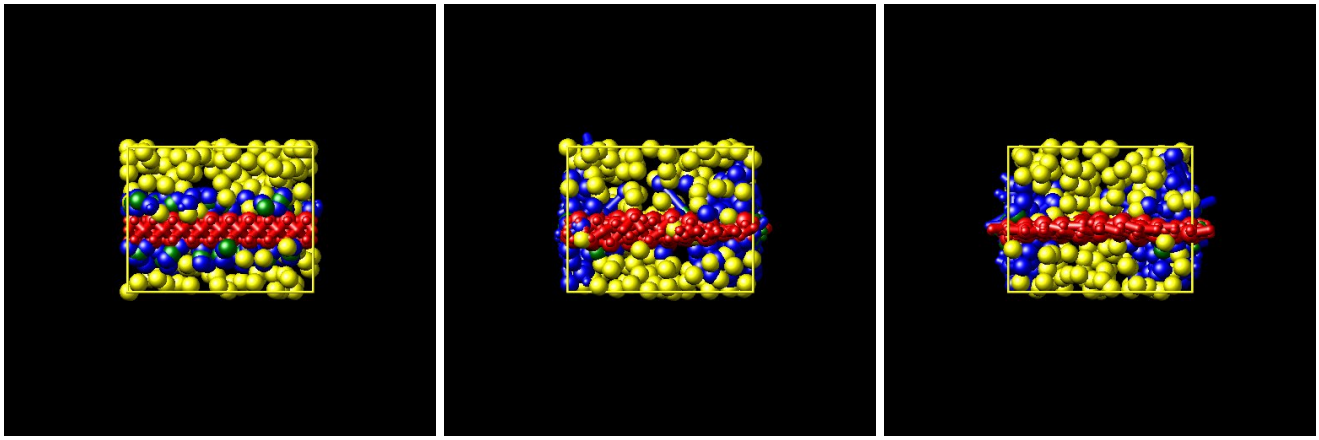
Figure 14

Sloghtly increase mod-mod repulsion
Sloghtly increase mod-poly repulsion

One-eight

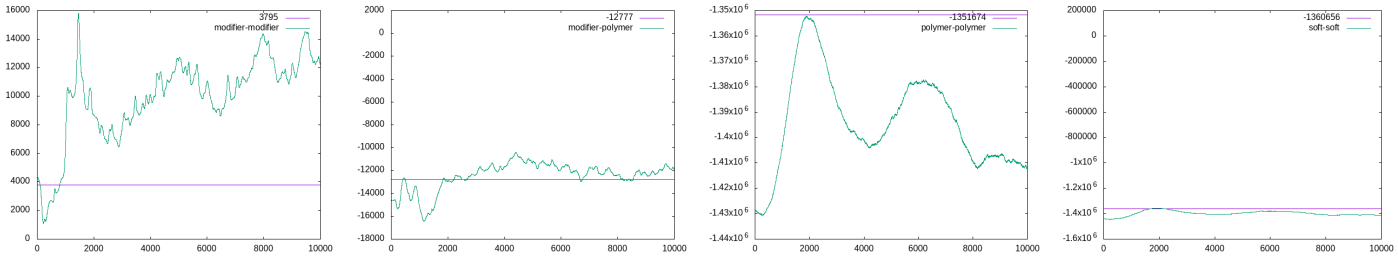
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.1
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=150, r=0.8	a=150, r=0.8	a=150, r=0.8
		a=150, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 15



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

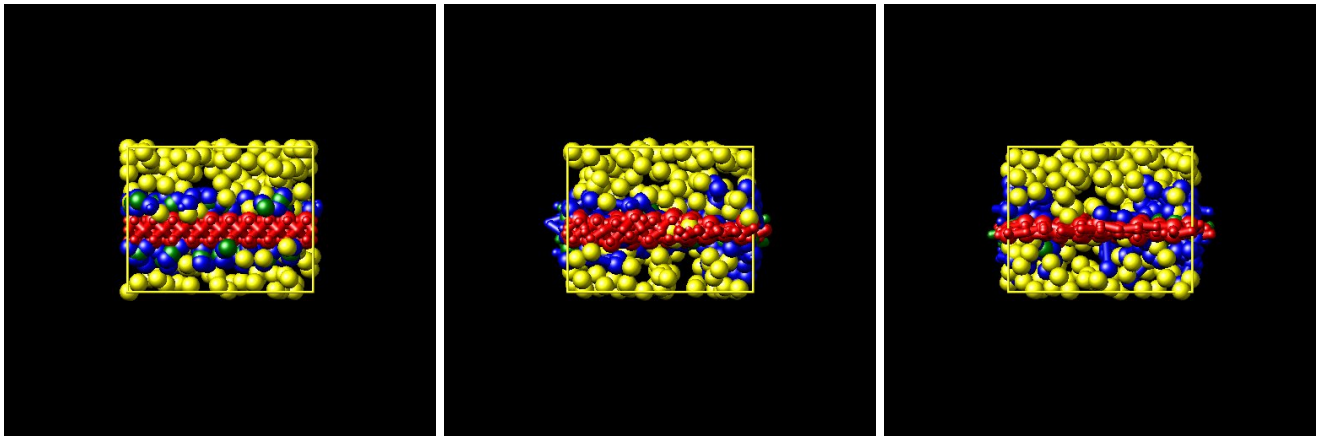
Figure 16

Decrease mod-mod repulsion
Decrease poly-poly attraction

One-nine

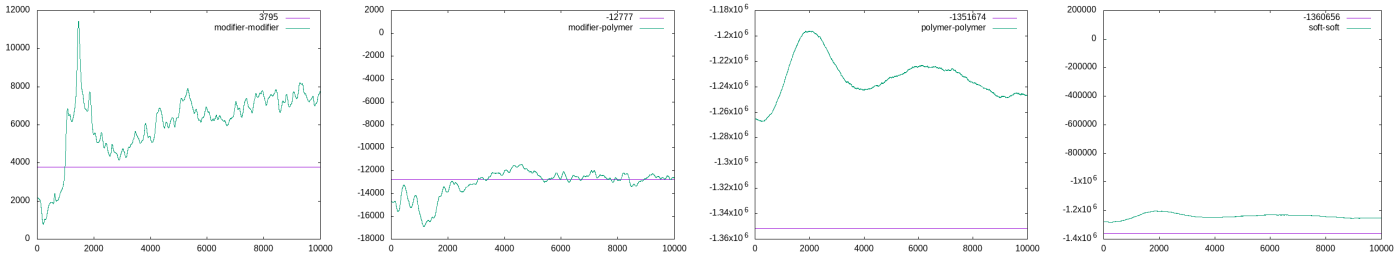
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.1
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.8 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=75, r=0.8	a=75, r=0.8	a=150, r=0.8
		a=75, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 17



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

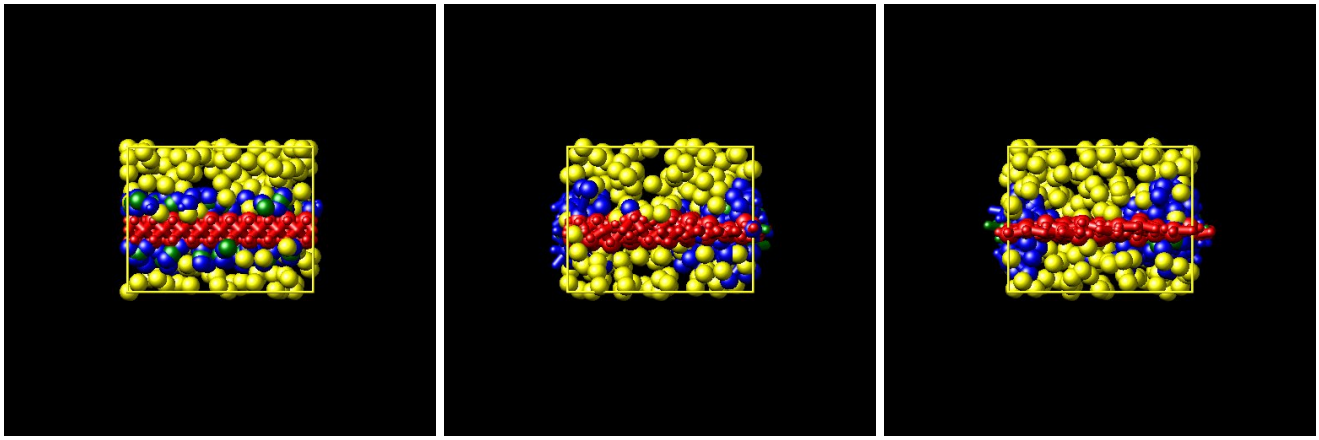
Figure 18

Slightly decrease mod-mod repulsion
Increase poly-poly attraction

One-ten

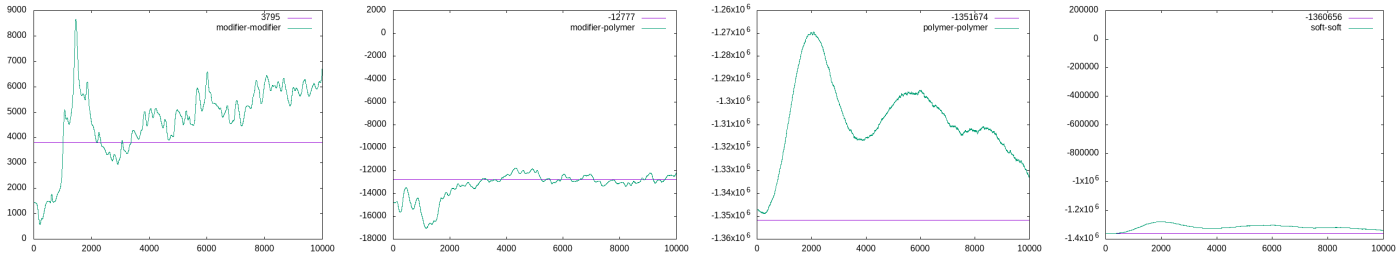
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.1
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=50, r=0.8	a=50, r=0.8	a=150, r=0.8
		a=50, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 19



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

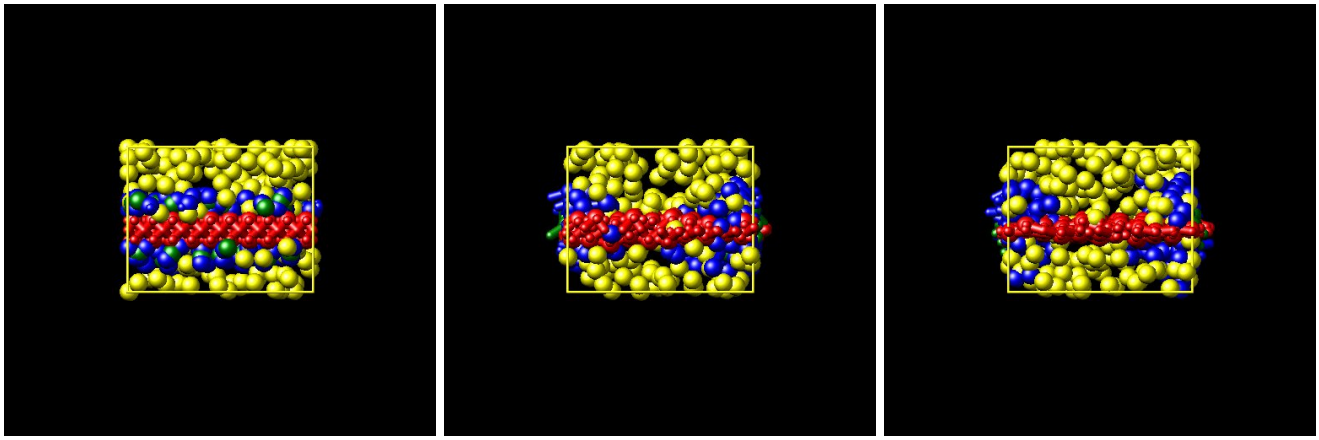
Figure 20

Slightly decrease mod-mod repulsion
Slightly increase poly-poly attraction

One-eleven

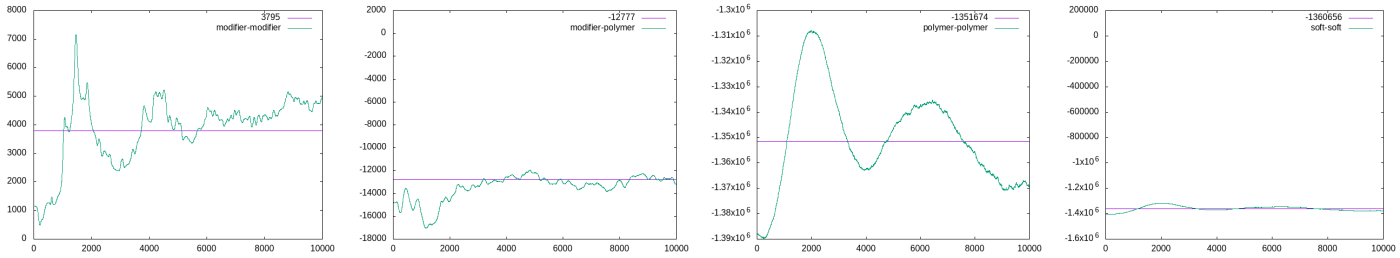
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 2 coul/cut/soft 0.1
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.875 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=500, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=40, r=0.8	a=40, r=0.8	a=150, r=0.8
		a=40, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 21



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

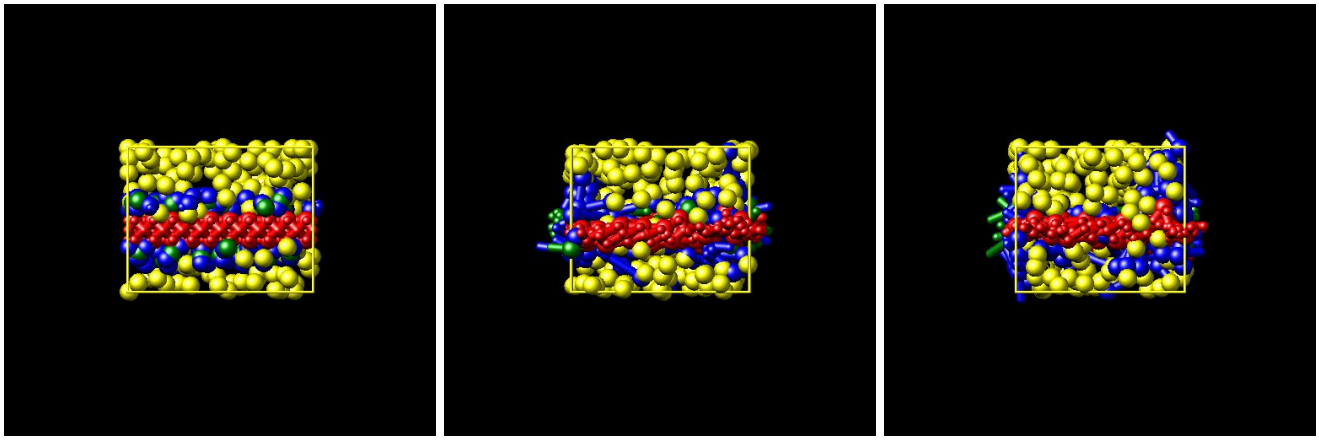
Figure 22

Slightly decrease mod-mod repulsion
Slightly increase poly-poly attraction

One-12

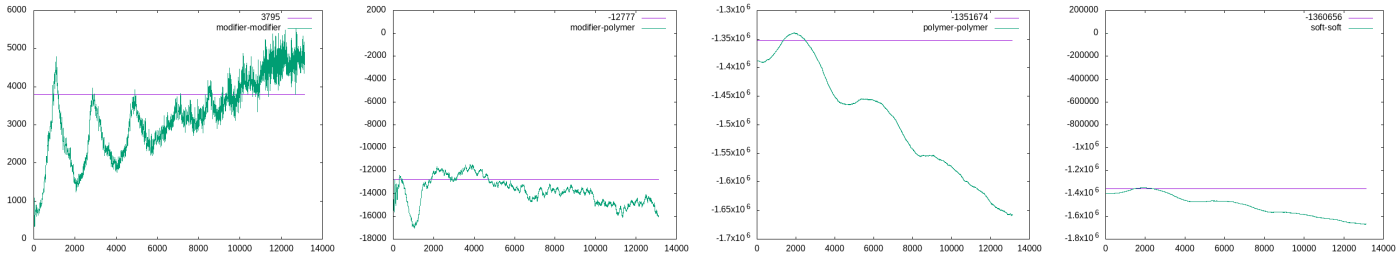
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.875 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=40, r=0.8	a=40, r=0.8	a=150, r=0.8
		a=40, r=1	a=150, r=1
			a=150, r=1



(a) (b) (c)

Figure 23



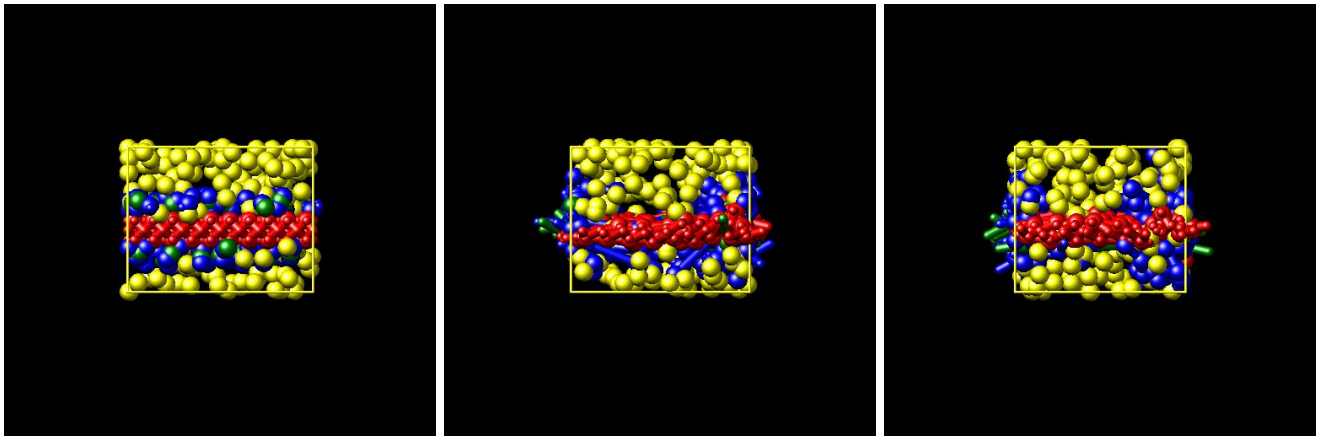
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 24

One-13

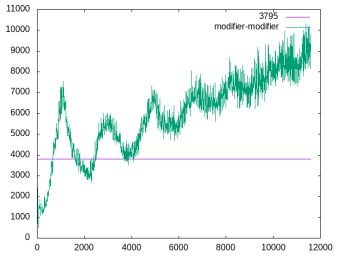
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=100, r=0.8	a=100, r=0.8	a=150, r=0.8
		a=40, r=1	a=250, r=1
			a=250, r=1

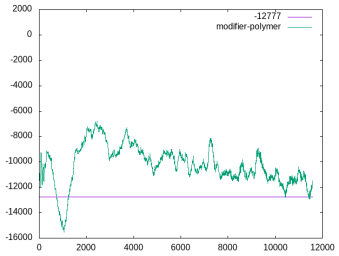


(a) (b) (c)

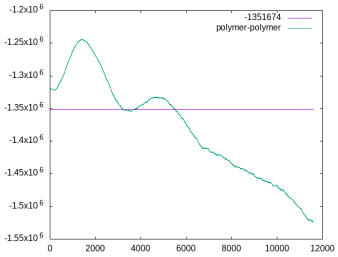
Figure 25



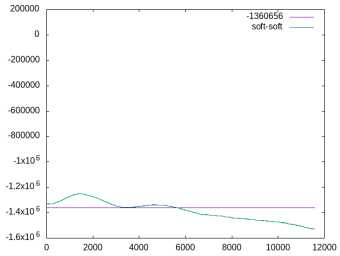
(a) mod-mod



(b) mod-poly



(c) poly-poly



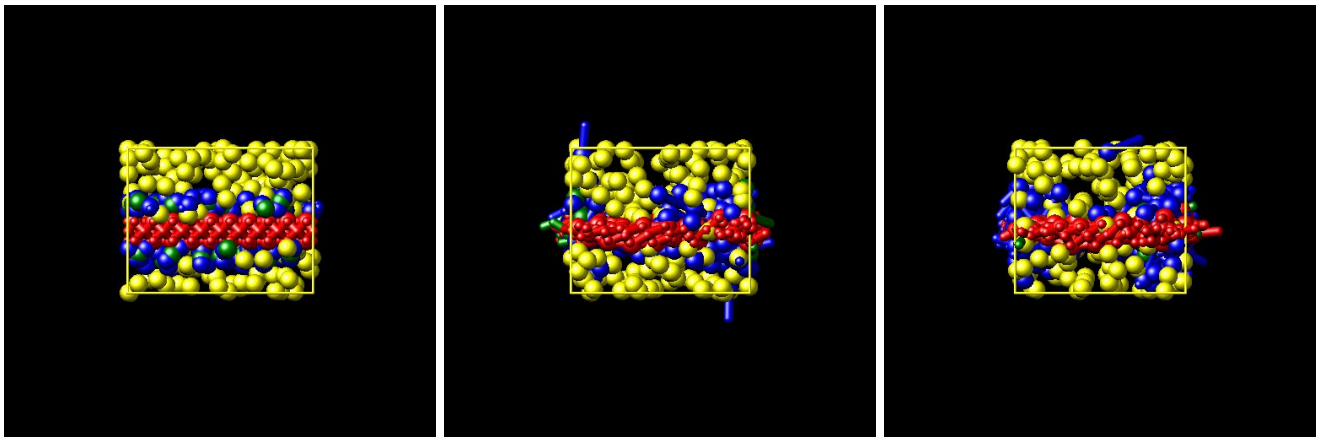
(d) soft-soft

Figure 26

One-14

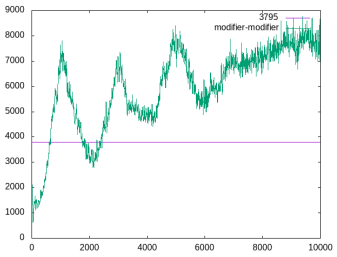
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=75, r=0.8	a=75, r=0.8	a=150, r=0.8
		a=75, r=1	a=250, r=1
			a=500, r=1

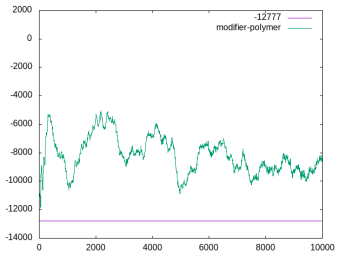


(a) (b) (c)

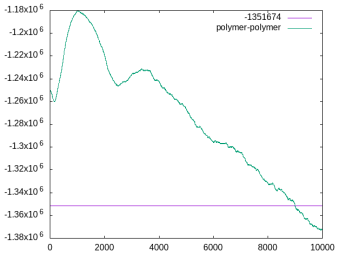
Figure 27



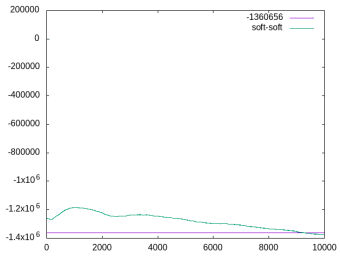
(a) mod-mod



(b) mod-poly



(c) poly-poly



(d) soft-soft

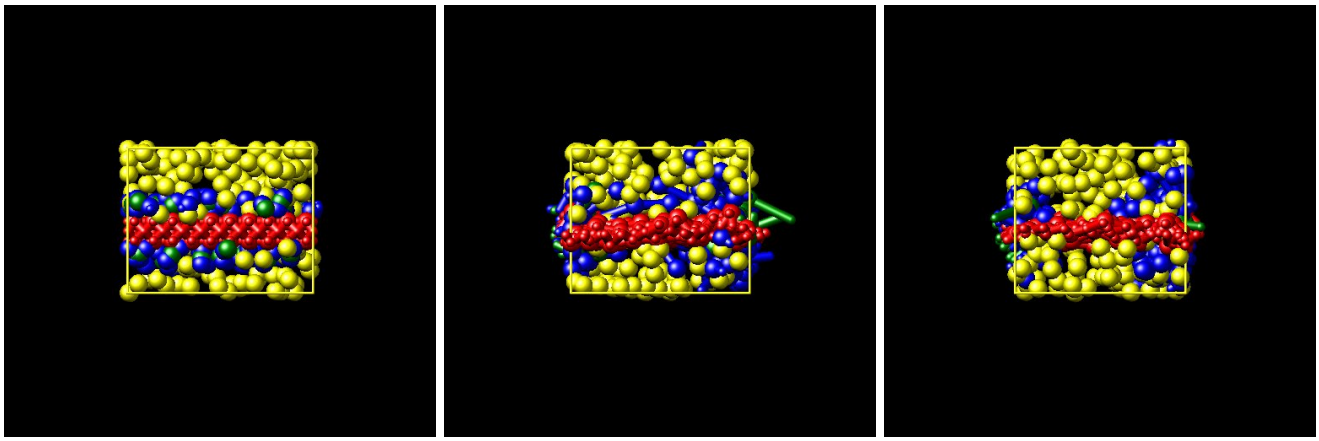
Figure 28

One-15

pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3

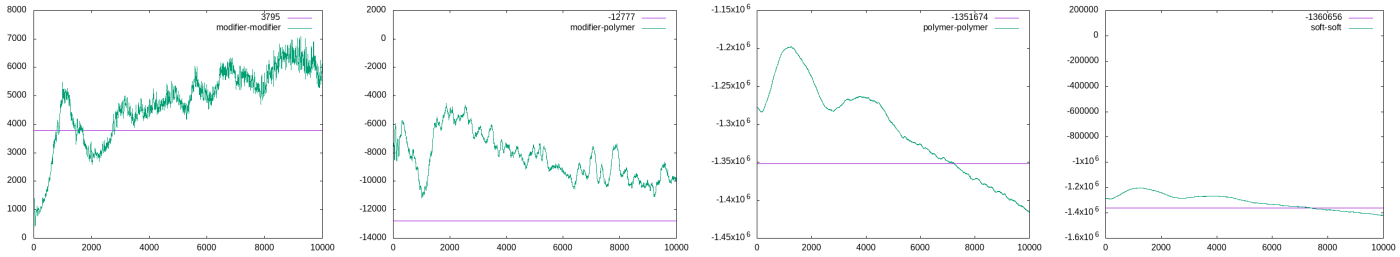
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=50, r=0.8	a=50, r=0.8	a=150, r=0.8
		a=50, r=1	a=350, r=1
			a=400, r=1



(a) (b) (c)

Figure 29



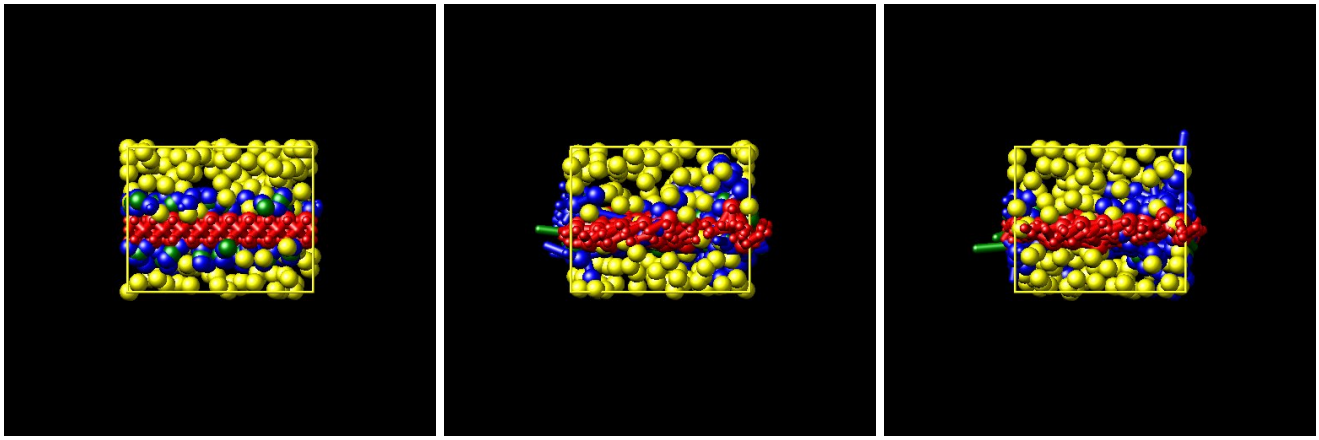
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 30

One-16

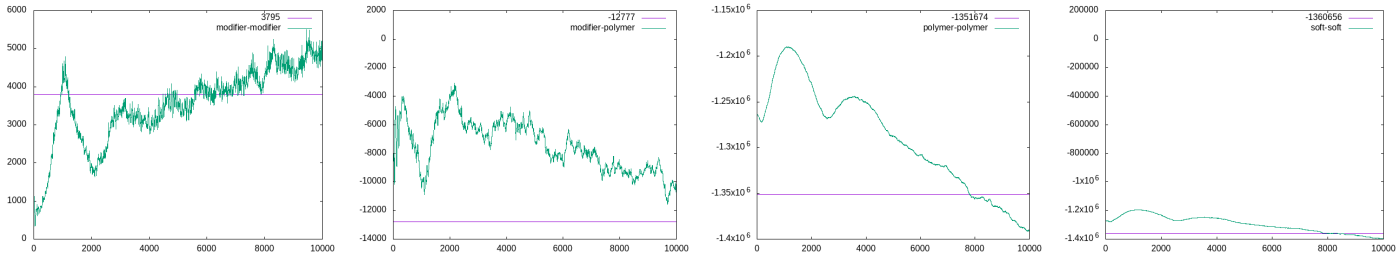
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=40, r=0.8	a=40, r=0.8	a=300, r=0.8
		a=40, r=1	a=300, r=1
			a=450, r=1



(a) (b) (c)

Figure 31



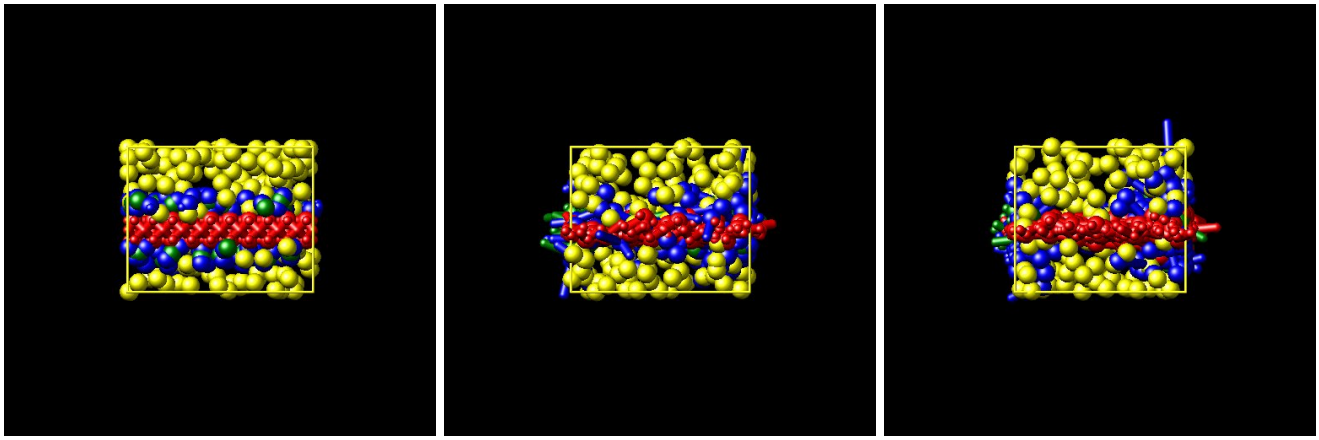
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 32

One-17 (==18?)

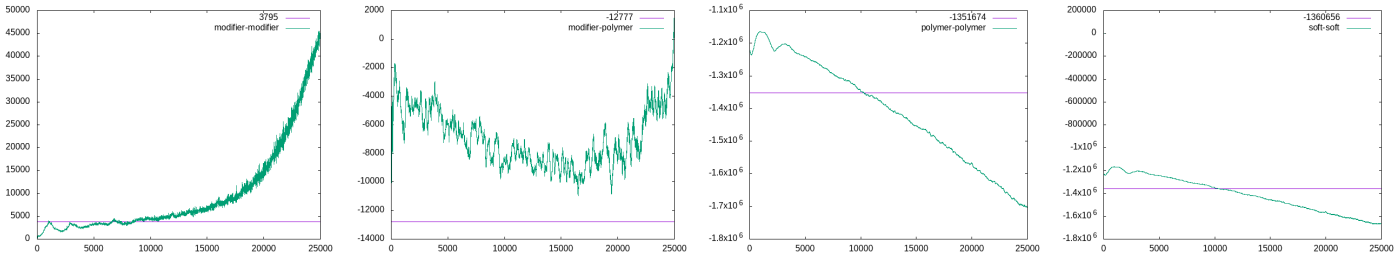
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=35, r=0.8	a=35, r=0.8	a=300, r=0.8
		a=35, r=1	a=300, r=1
			a=600, r=1



(a) (b) 5k (c) 10k

Figure 33



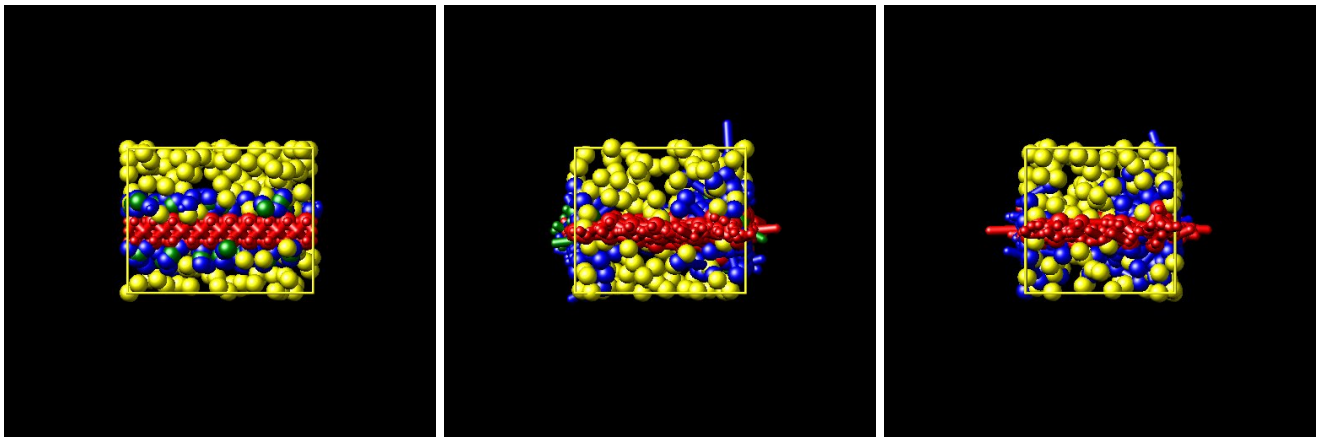
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 34

One-18

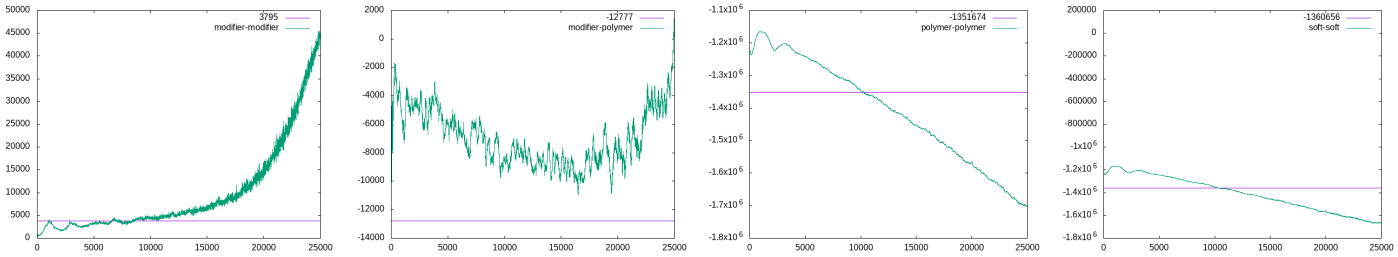
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=35, r=0.8	a=35, r=0.8	a=300, r=0.8
		a=35, r=1	a=300, r=1
			a=600, r=1



(a) (b) 10k (c) 25k

Figure 35



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

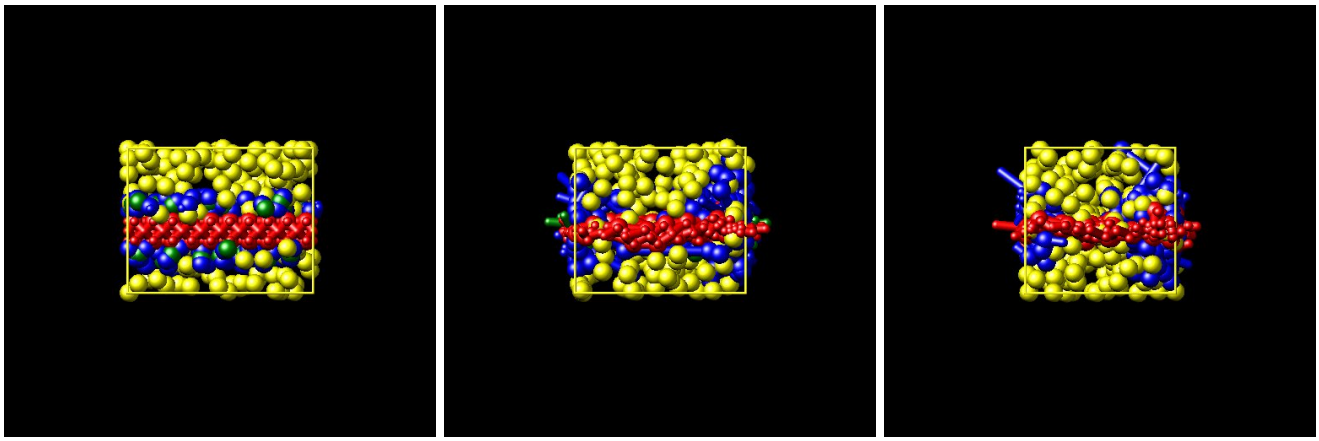
Figure 36

One-19

pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3

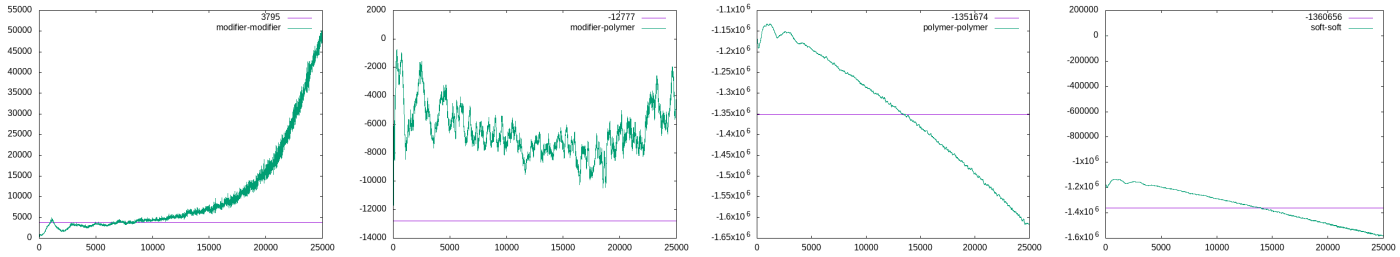
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=40, r=0.8	a=40, r=0.8	a=300, r=0.8
		a=40, r=1	a=250, r=1
			a=800, r=1



(a) (b) 10k (c) 25k

Figure 37



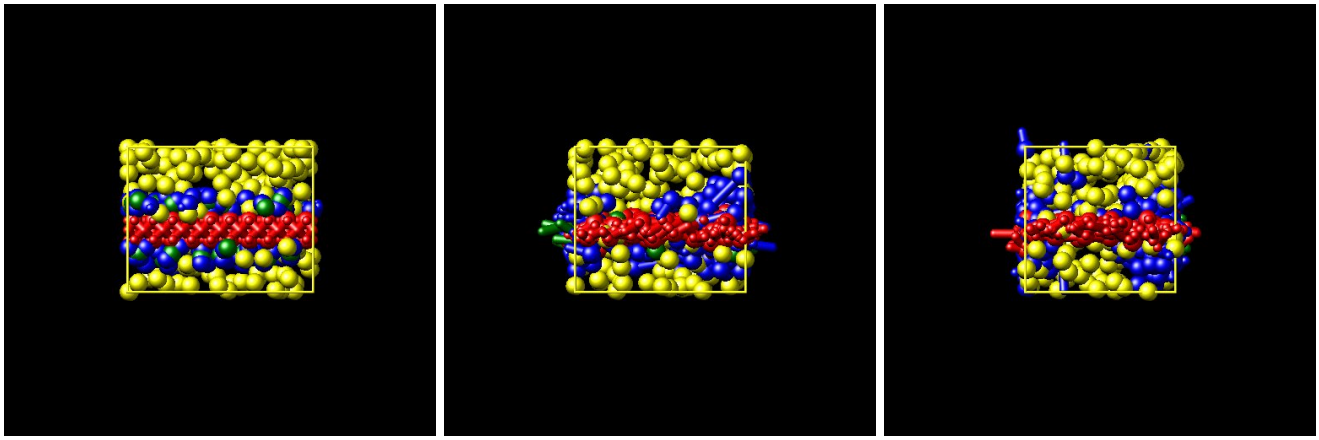
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 38

One-20

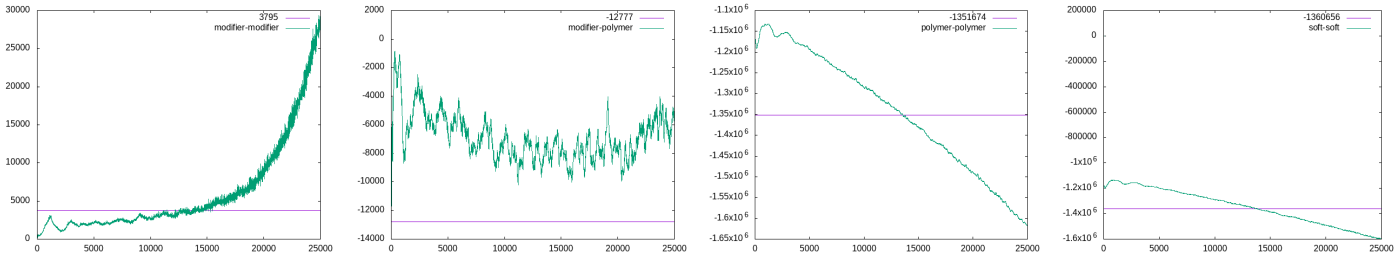
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=300, r=0.8
		a=25, r=1	a=250, r=1
			a=800, r=1



(a) (b) 10k (c) 25k

Figure 39



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

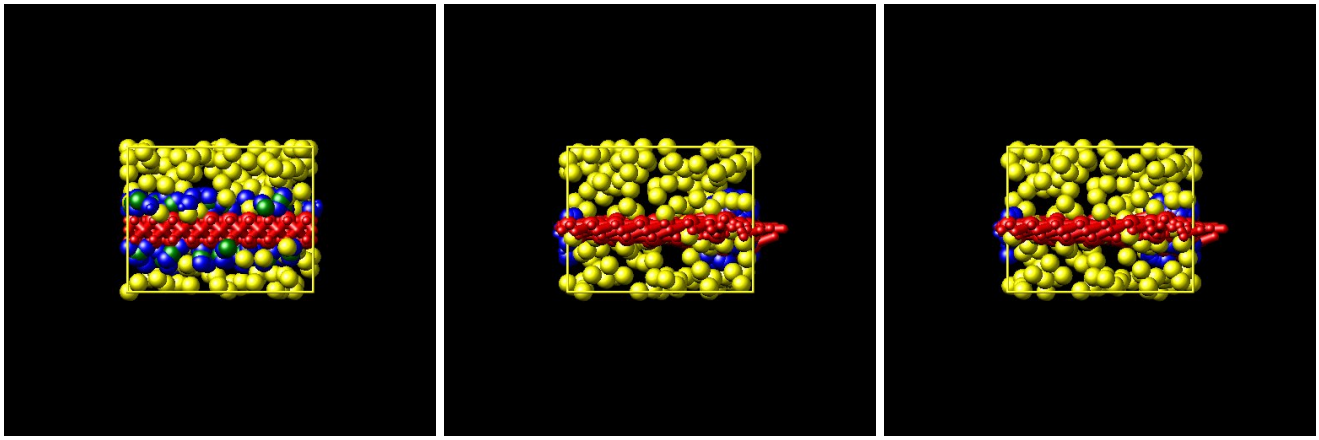
Figure 40

NVT

One-21

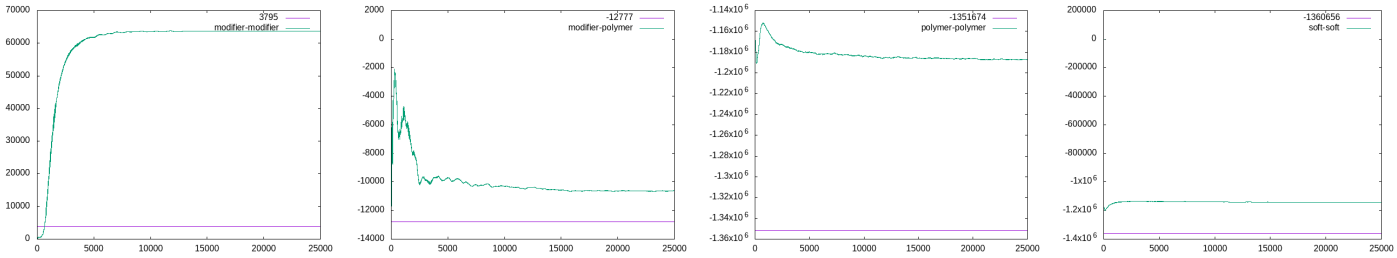
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=300, r=0.8
		a=25, r=1	a=250, r=1
			a=800, r=1



(a) (b) 10k (c) 25k

Figure 41



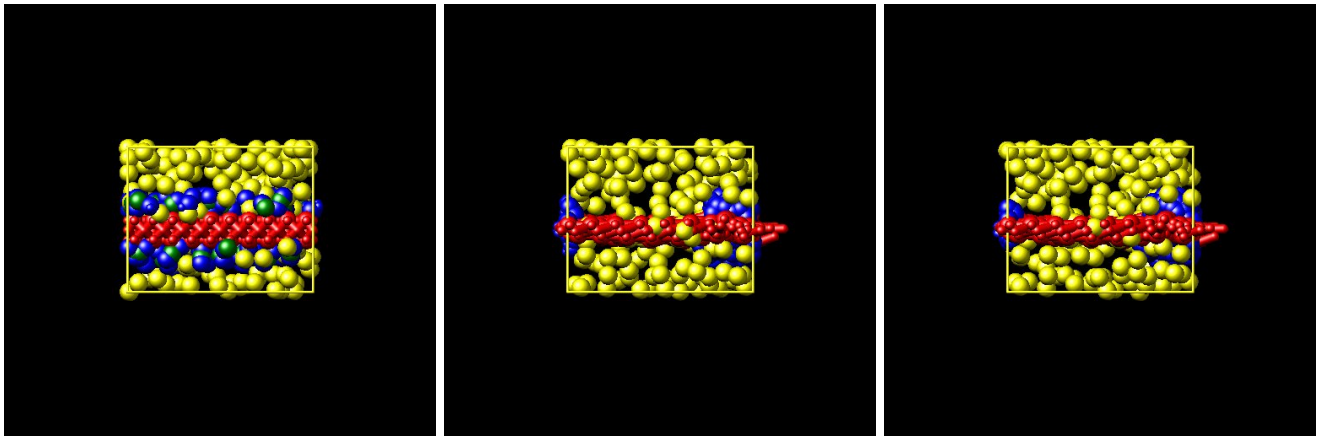
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 42

One-22

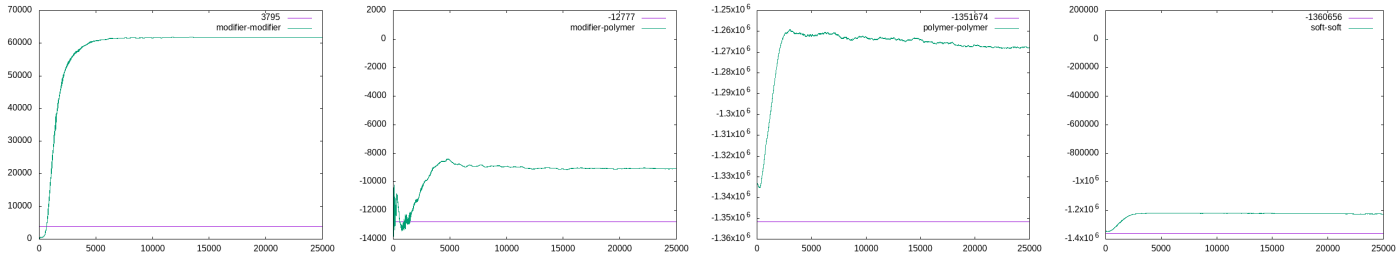
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 4 lj/cut/soft 0.07 10 3 3
pair_coeff 4 4 lj/cut/soft 0.85 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 10k (c) 25k

Figure 43



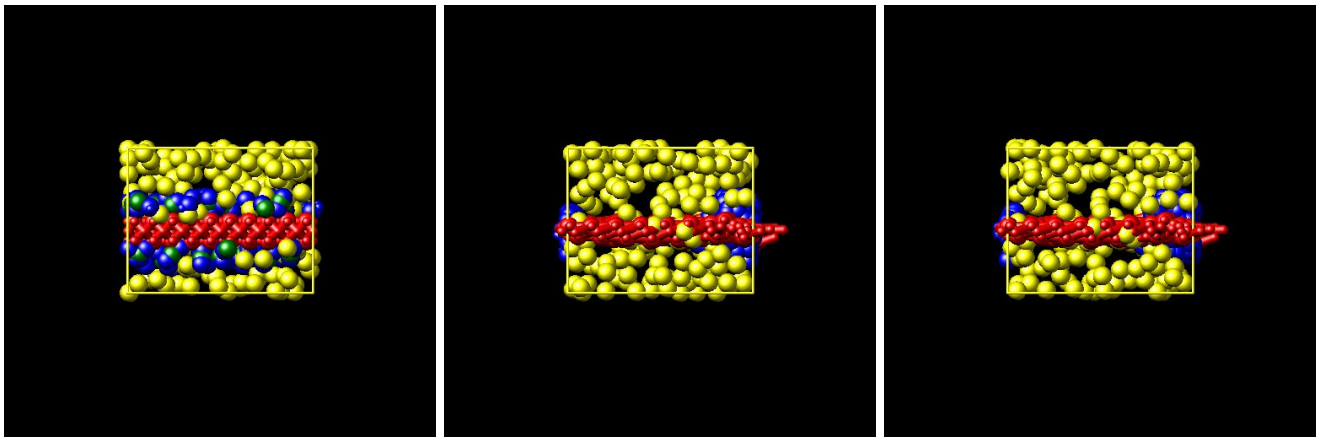
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 44

One-23

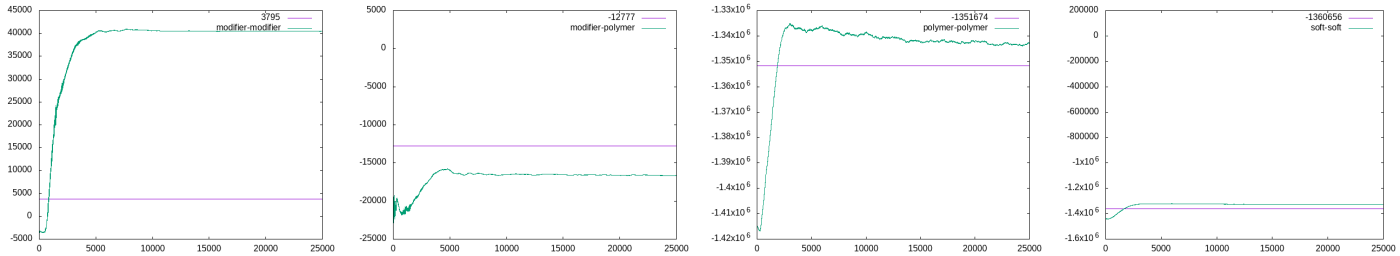
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 3 lj/cut/soft 0.15 10 3 3
pair_coeff 3 4 lj/cut/soft 0.1 10 3 3
pair_coeff 4 4 lj/cut/soft 0.9 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 10k (c) 25k

Figure 45



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

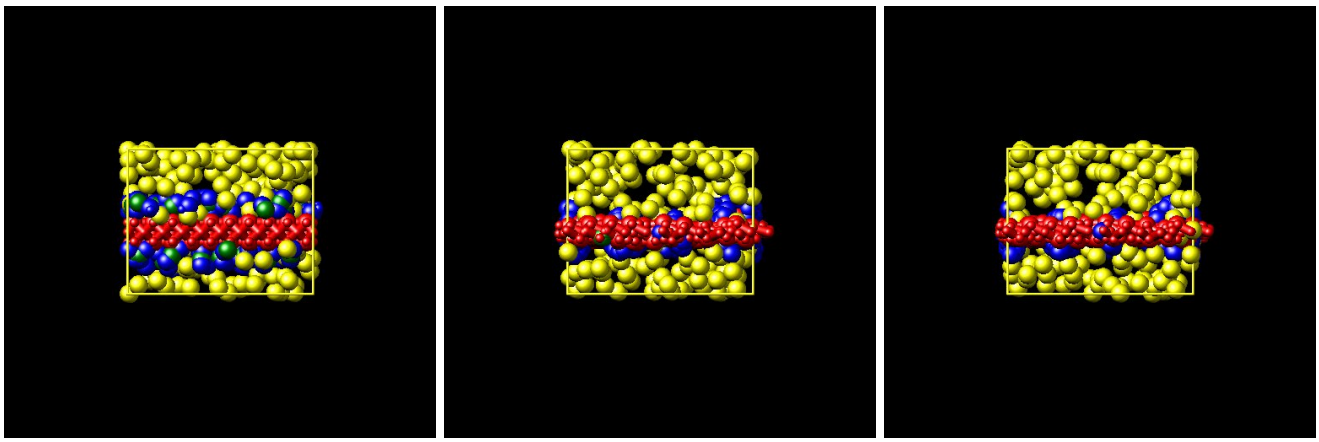
Figure 46

One-25

pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/cut/soft 0.25 pair_coeff 1 2 coul/cut/soft 0.5
pair_coeff 3 3 lj/cut/soft 0.25 10 3 3

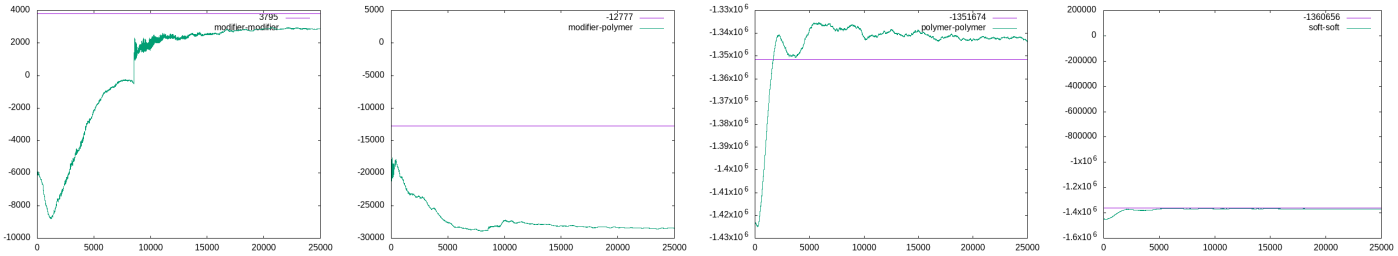
pair_coeff 3 4 lj/cut/soft 0.095 10 3 3
pair_coeff 4 4 lj/cut/soft 0.905 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=0.8	a=500, r=0.8	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 10k (c) 25k

Figure 47



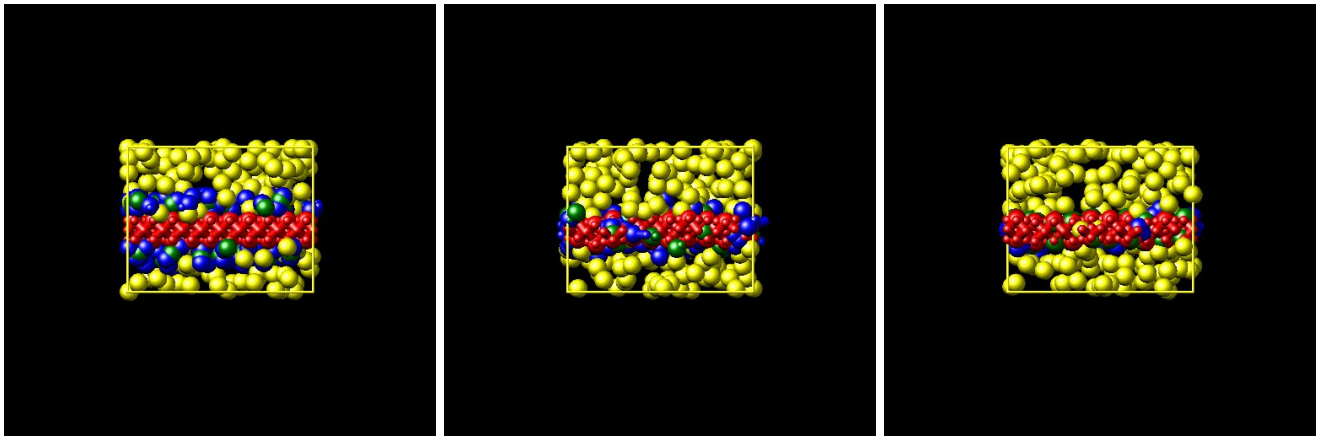
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 48

One-25

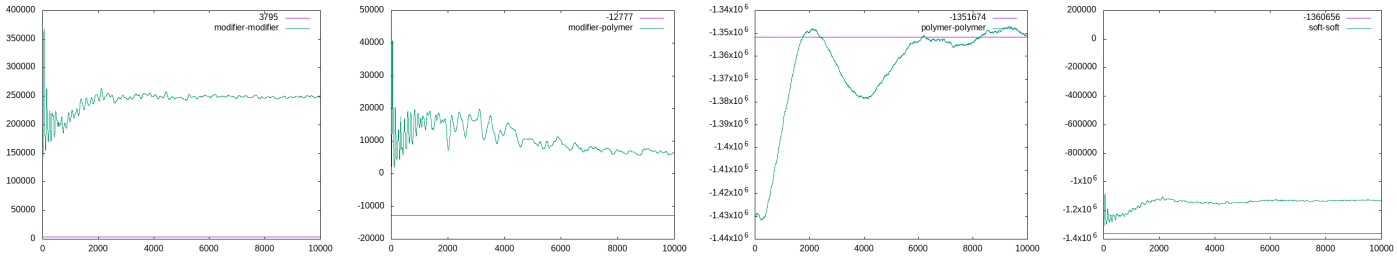
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/long/soft 0.25
pair_coeff 1 2 coul/long/soft 0.25
pair_coeff 2 2 coul/long/soft 0.25
pair_coeff 3 3 lj/cut/soft 0.25 10 3 3
pair_coeff 3 4 lj/cut/soft 0.0925 10 3 3
pair_coeff 4 4 lj/cut/soft 0.910 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=1.2	a=500, r=0.8	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 5k (c) 10k

Figure 49



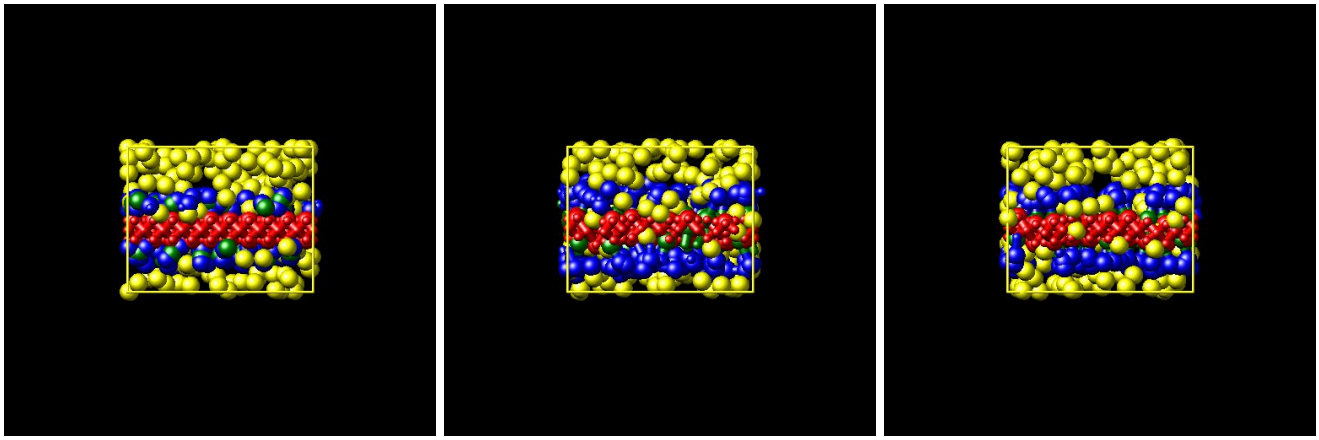
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 50

One-27

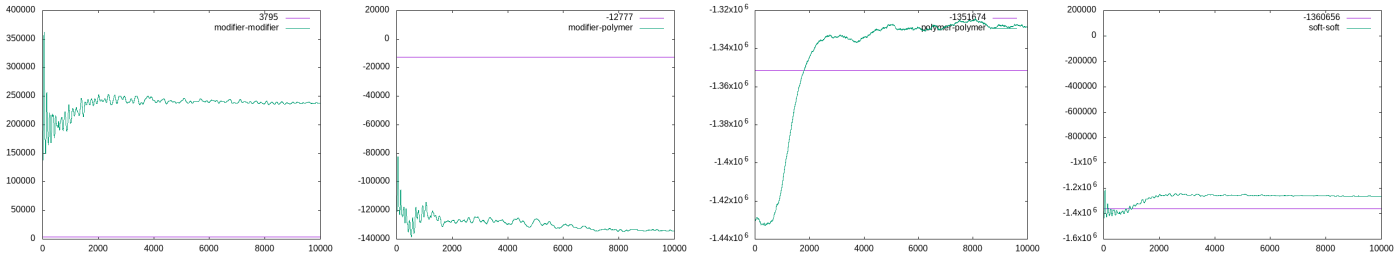
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/long/soft 0.25
pair_coeff 1 2 coul/long/soft 0.25
pair_coeff 2 2 coul/long/soft 0.25
pair_coeff 3 3 lj/cut/soft 0.5 10 3 3
pair_coeff 3 4 lj/cut/soft 0.5 10 3 3
pair_coeff 4 4 lj/cut/soft 0.910 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=1.5	a=500, r=1.5	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 5k (c) 10k

Figure 51



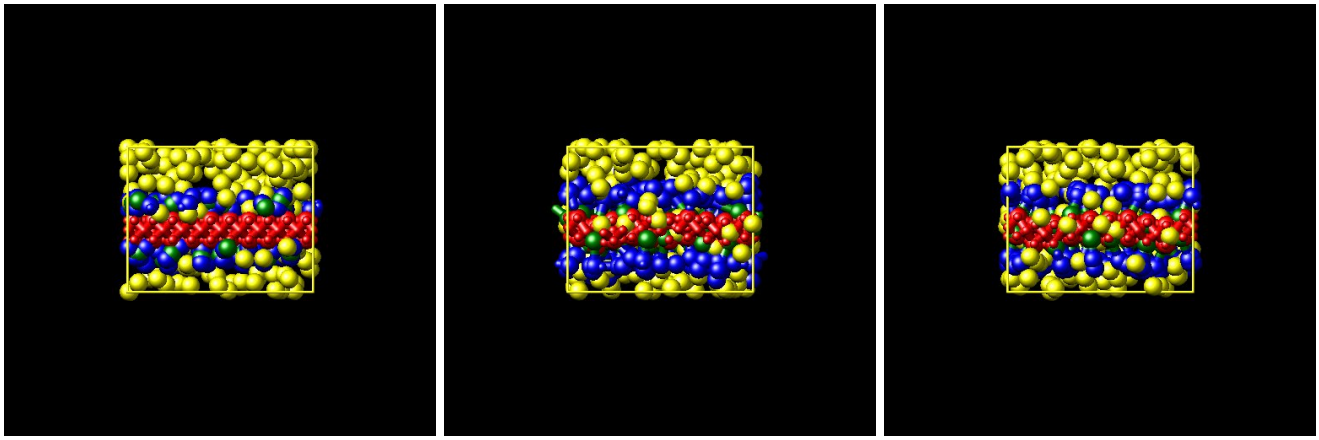
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 52

One-27

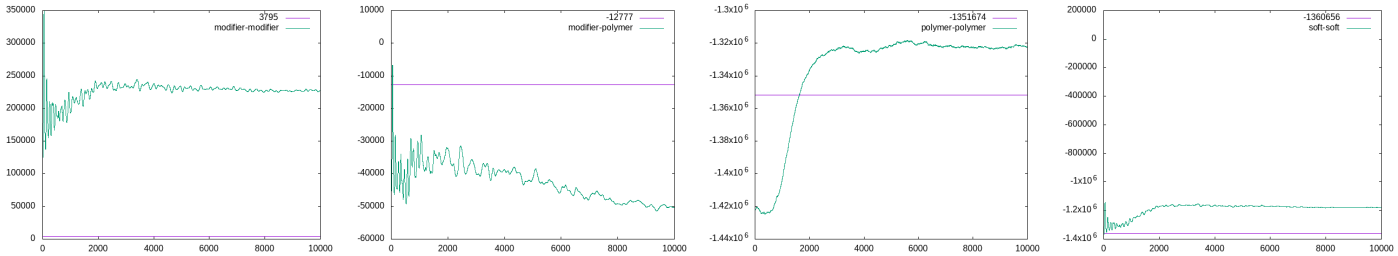
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/long/soft 0.25
pair_coeff 1 2 coul/long/soft 0.25
pair_coeff 2 2 coul/long/soft 0.25
pair_coeff 3 3 lj/cut/soft 1.0 10 3 3
pair_coeff 3 4 lj/cut/soft 0.25 10 3 3
pair_coeff 4 4 lj/cut/soft 0.905 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=1.5	a=500, r=1.5	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 5k (c) 10k

Figure 53



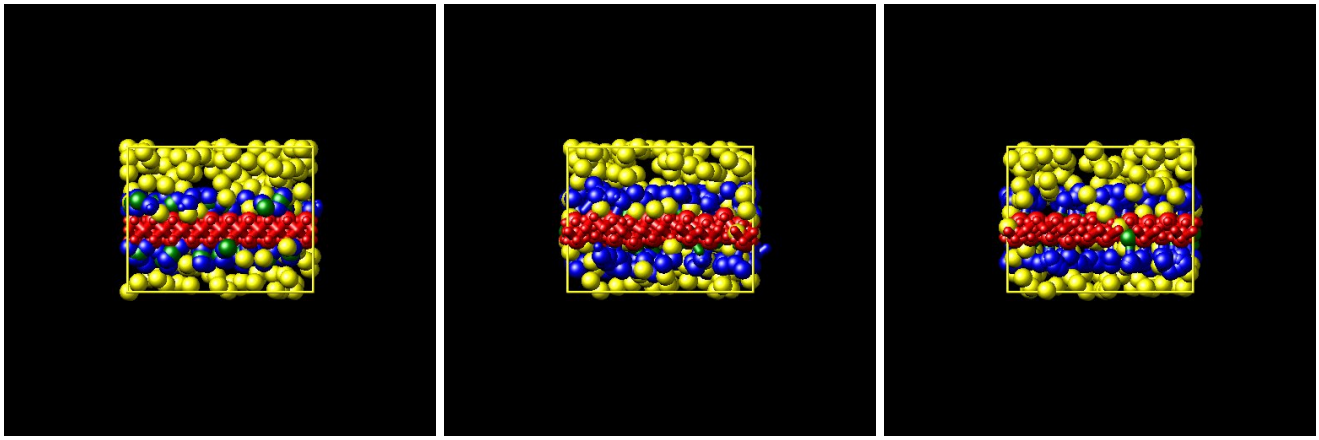
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 54

One-29

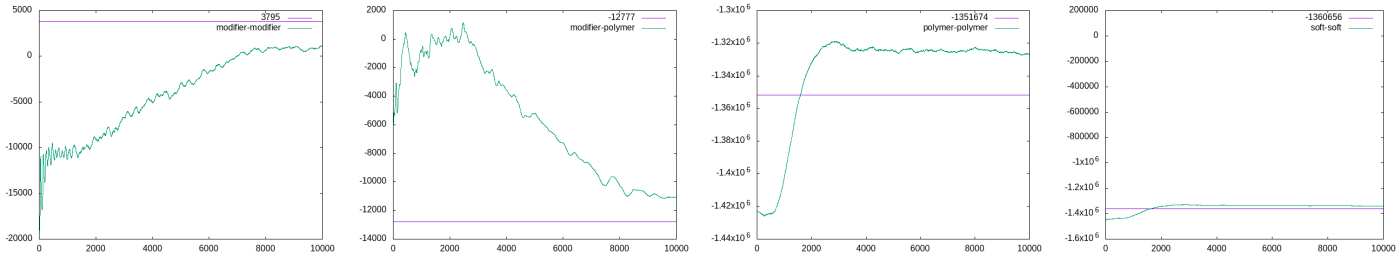
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/long/soft 0.25
pair_coeff 1 2 coul/long/soft 0.25
pair_coeff 2 2 coul/long/soft 0.25
pair_coeff 3 3 lj/cut/soft 1.0 10 3 3
pair_coeff 3 4 lj/cut/soft 0.05 10 3 3
pair_coeff 4 4 lj/cut/soft 0.905 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=500, r=1.5	a=500, r=1.5	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 5k (c) 10k

Figure 55



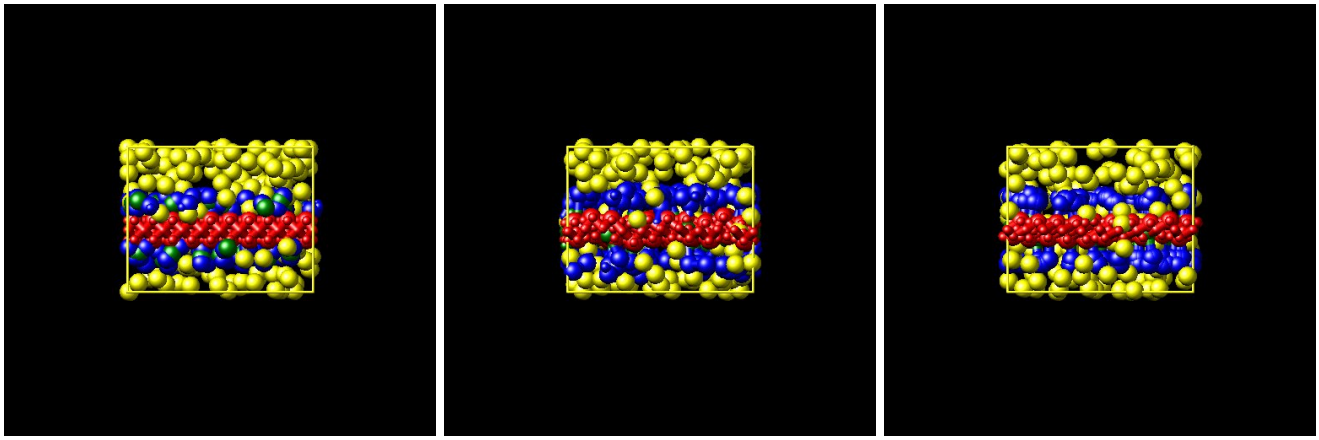
(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 56

One-30

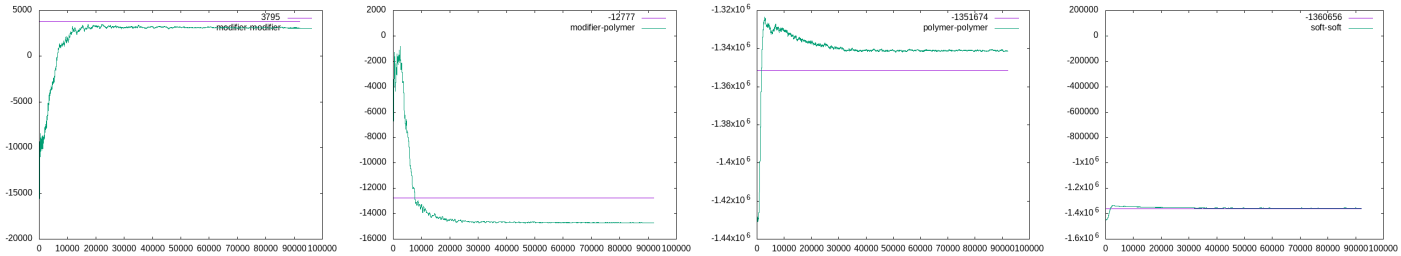
pair_style hybrid/overlay dpd 1 1 34387 & coul/cut/soft 2 1 5 & lj/cut/soft 2 1 5
pair_coeff 1 1 coul/long/soft 0.25
pair_coeff 1 2 coul/long/soft 0.25
pair_coeff 2 2 coul/long/soft 0.05
pair_coeff 3 3 lj/cut/soft 0.95 10 3 3
pair_coeff 3 4 lj/cut/soft 0.055 10 3 3
pair_coeff 4 4 lj/cut/soft 0.908 10 3 3
DPD coefficients: a_{ij} and r_c

MMT	Head	Tail	Polymer
a=50000, r=0.95	a=50000, r=1.5	a=500, r=1.5	a=500, r=0.8
	a=25, r=0.8	a=25, r=0.8	a=200, r=0.8
		a=25, r=1	a=200, r=1
			a=200, r=1



(a) (b) 5k (c) 10k

Figure 57



(a) mod-mod (b) mod-poly (c) poly-poly (d) soft-soft

Figure 58