Thermodynamics signature of structural transitions and dissociation of charged colloidal clusters: a parallel tempering Monte Carlo study

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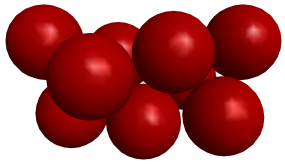
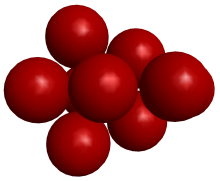
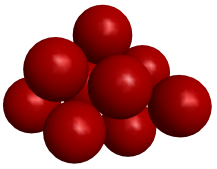
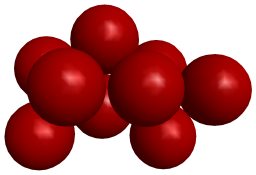
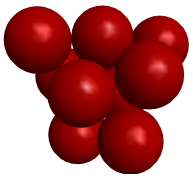
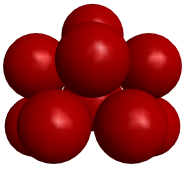
Table S1. Energy range of the structures from Set I, Set II, and Set III for each cluster size. For the Set I of *N*=17 and *N*=18, there is only one structure whose energy is indicated.

N	**Set I**	**Set II**	**Set III**
9	(−15.562,−15.290)	(−10.790,−9.372)	(−7.558,−4.702)
10	(−17.211,−16.581)	(−13.885,−9.810)	(−8.922,−5.168)
11	(−18.091,−17.748)	(−15.516,−10.261)	(−8.472,−5.632)
12	(−19.338,−18.580)	(−16.356,−10.717)	(−8.933,−6.096)
17	−24.198	(−23.181,−17.634)	(−10.183,−8.414)
18	−25.108	a: (−24.538,−22.779)	(−10.646,−8.877)
		b: (−21.826,−18.099)	
19	(−26.154,−24.902)	a: (−24.332,−22.304)	(−11.109,−9.304)
		b:(−21.208,−16.785)	
20	(−27.291,−26.296)	a: (−25.773,−22.774)	(−11.572,−9.804)
		b: (−21.657,−19.027)	

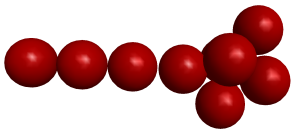
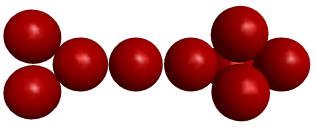
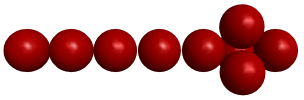
Small clusters data

N=9

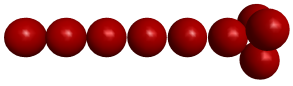
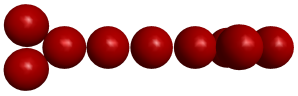
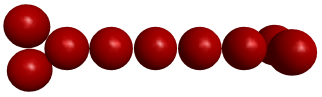
SET I:

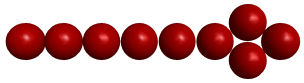
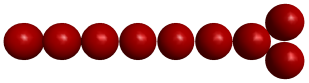
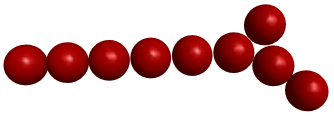
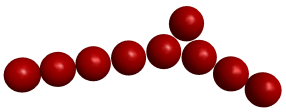
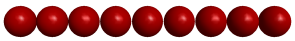
9A Energy: -15.56156020 	9B Energy: -15.55806630 	9C Energy: -15.46152621 
9D Energy: -15.37419913 	9E Energy: -15.35417435 	9F Energy: -15.28992983 

SET II

9G Energy: -10.78993014 	9H Energy: -10.21788243 	9I Energy: -9.37254143 

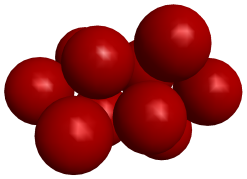
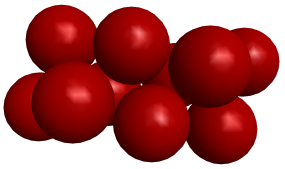
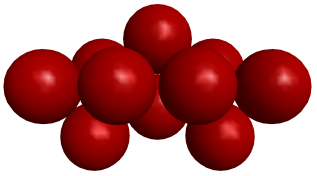
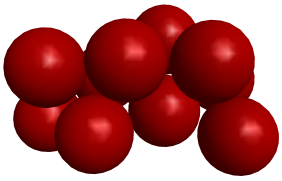
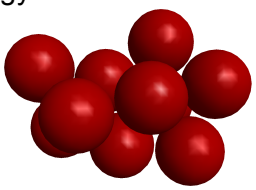
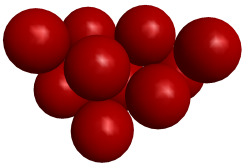
SET III

9J Energy: -7.55783121 	9K Energy: -7.39310189 	9L Energy: -6.54710392 

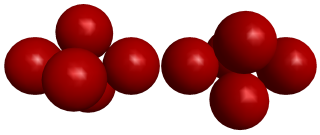
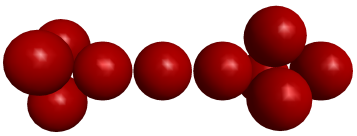
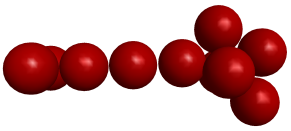
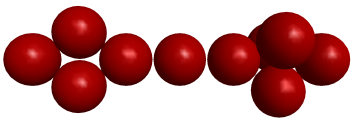
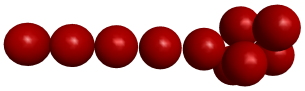
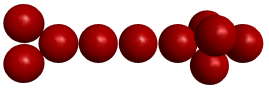
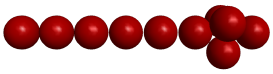
9M Energy: -6.48545675 	9N Energy: -5.62736246 	9O Energy: -5.24671446 
9P Energy: -5.10267896 	9Q Energy: -4.70201501 	

N=10

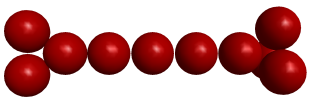
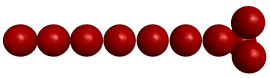
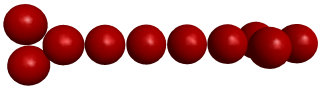
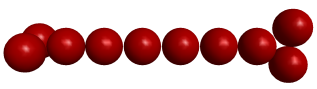
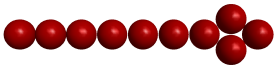
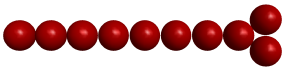
SET I

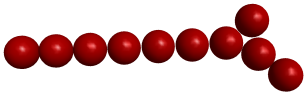
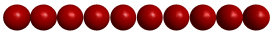
10A Energy: -17.21101095 	10B Energy: -16.87425093 	10C Energy: -16.68045730 
10D Energy: -16.64222794 	10E Energy: -16.62190950 	10F Energy: -16.58118497 

SET II

10G Energy: -13.88520948 	10H Energy: -12.46579791 	10I Energy: -12.00287046 
10J Energy: -11.46719574 	10K Energy: -11.18262418 	10L Energy: -10.69663547 
10M Energy: -9.81047846 		

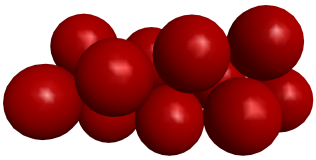
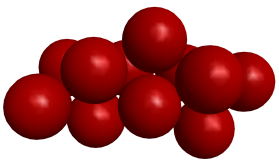
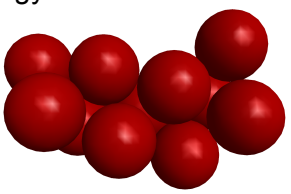
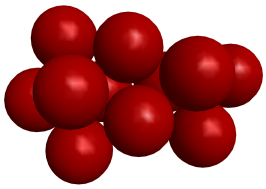
SET III

10N Energy: -8.92247264 	10O Energy: -8.01291959 	10P Energy: -7.85884213 
10Q Energy: -7.01105861 	10R Energy: -6.94437832 	10S Energy: -6.09081450 

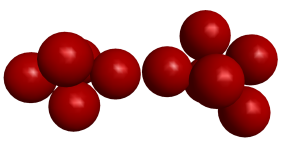
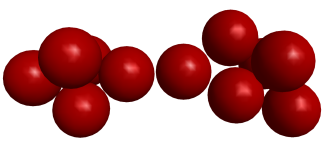
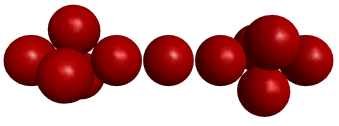
10T Energy: -5.70562160 	10U Energy: -5.16777479 	

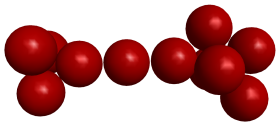
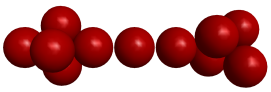
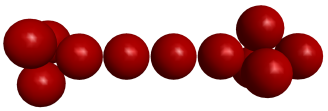
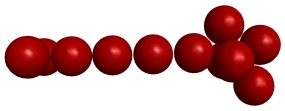
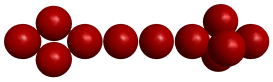
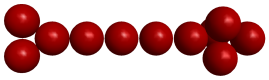
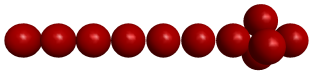
N=11

SET I

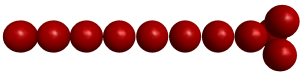
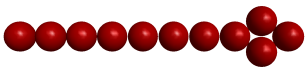
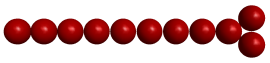
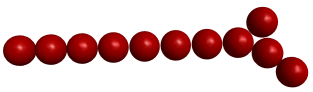
11A Energy: -18.09068047 	11B Energy: -17.85065043 	11C Energy: -17.80311256 
11D Energy: -17.74788989 		

SET II

11E Energy: -15.51605893 	11F Energy: -14.78362454 	11G Energy: -14.64097653 

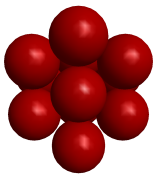
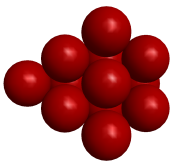
11H Energy: -14.20555101 	11I Energy: -13.57236423 	11J Energy: -13.01227628 
11K Energy: -12.48451081 	11L Energy: -11.97787636 	11M Energy: -11.16475660 
11N Energy: -10.26084011 		

SET III

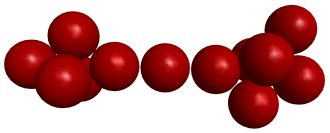
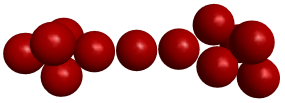
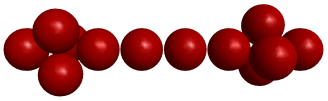
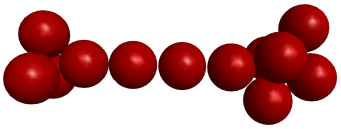
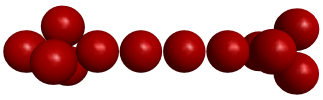
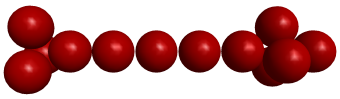
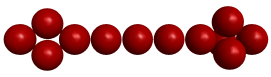
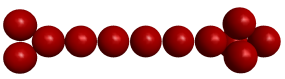
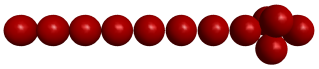
11O Energy: -8.47198864 	11P Energy: -7.40544575 	11Q Energy: -6.55424225 
11R Energy: -6.16667287 	11S Energy: -5.63242993 	

N=12

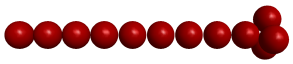
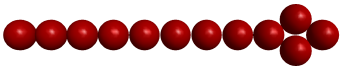
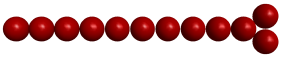
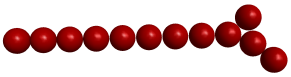
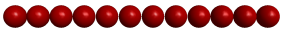
SET I

12A Energy: -19.33769398 	12B Energy: -18.58018841 	

SET II

12C Energy: -16.35607159 	12D Energy: -15.51831926 	12E Energy: -15.22193037 
12F Energy: -14.77758078 	12G Energy: -14.12146597 	12H Energy: -13.51098250 
12I Energy: -12.46106057 	12J Energy: -11.62952326 	12K Energy: -10.71737568 

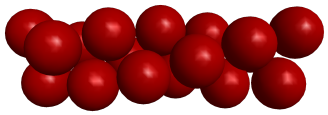
SET III

12L Energy: -8.93305764 	12M Energy: -7.86757644 	12N Energy: -7.01762623 
12O Energy: -6.62879110 	12P Energy: -6.09647630 	

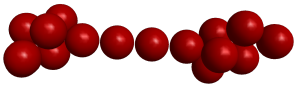
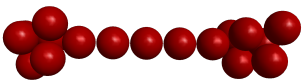
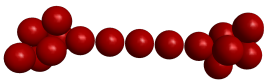
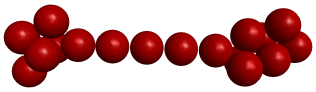
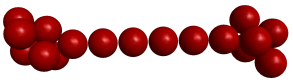
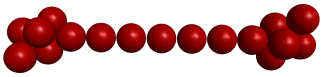
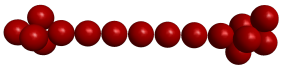
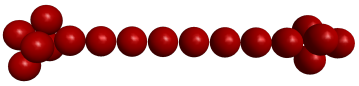
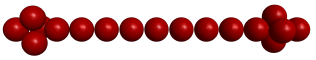
Larger clusters data

N=17

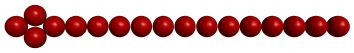
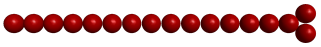
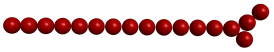
SET I

17A Energy: -24.19775922 		

SET II

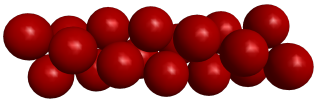
17B Energy: -23.18147845 	17C Energy: -22.36142585 	17D Energy: -22.36142245 
17E Energy: -22.25523432 	17F Energy: -21.33582304 	17G Energy: -20.26432848 
17H Energy: -20.04639508 	17I Energy: -18.95418110 	17J Energy: -17.63445734 

SET III

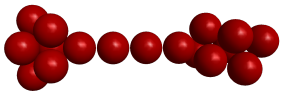
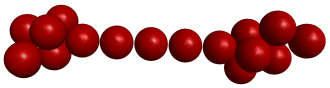
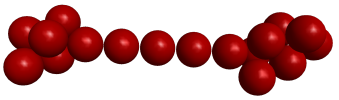
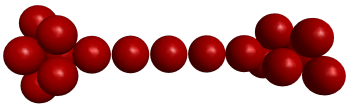
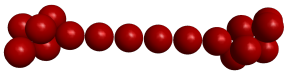
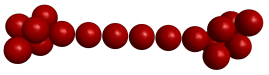
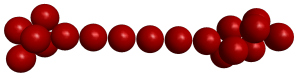
17K Energy: -10.18269373 	17L Energy: -9.33416592 	17M Energy: -8.94388763 
17N Energy: -8.41378484 		

N=18

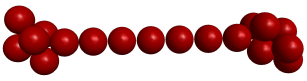
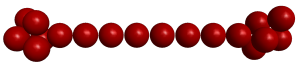
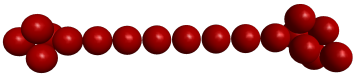
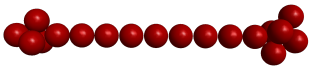
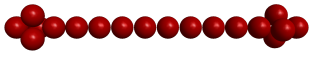
SET I

18A Energy: -25.10845390 		

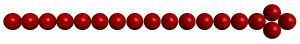
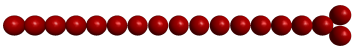
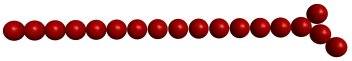
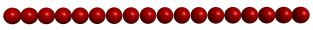
SET IIa

18B Energy: -24.53813820 	18C Energy: -23.79528244 	18D Energy: -23.79528024 
18E Energy: -23.75460477 	18F Energy: -22.89050733 	18G Energy: -22.89050611 
18H Energy: -22.77932744 		

SET IIb

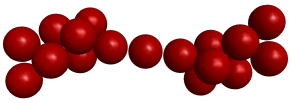
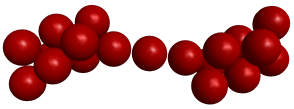
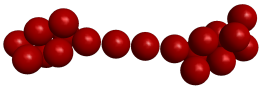
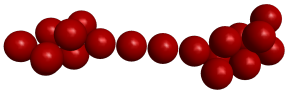
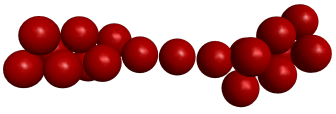
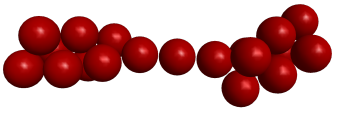
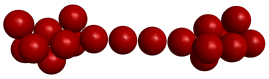
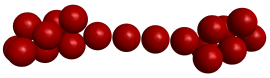
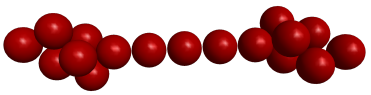
18I Energy: -21.82630174 	18J Energy: -20.73902524 	18K Energy: -20.51963552 
18L Energy: -19.42168115 	18M Energy: -18.09930357 	

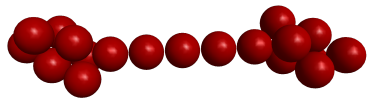
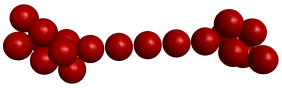
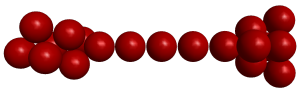
SET III

18N Energy: -10.64593661 	18O Energy: -9.79744424 	18P Energy: -9.40712976 
18Q Energy: -8.87708291 		

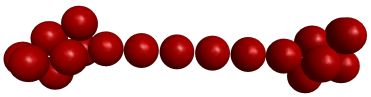
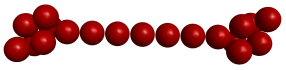
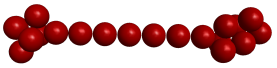
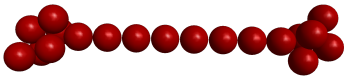
N=19

SET I

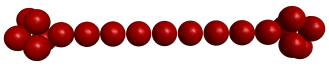
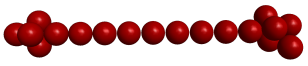
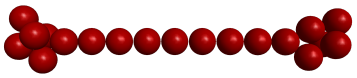
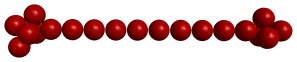
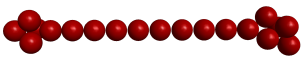
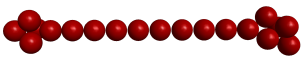
19A Energy: -26.15384179 	19B Energy: -26.15380677 	19C Energy: -25.82448915 
19D Energy: -25.82448293 	19E Energy: -25.77530111 	19F Energy: -25.77528932 
19G Energy: -25.64763543 	19H Energy: -25.32602688 	19I Energy: -25.22691019 

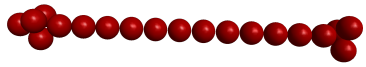
19J Energy: -25.22690894 	19K Energy: -25.04443432 	19L Energy: -24.90223850 

SET IIa

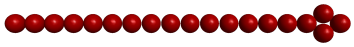
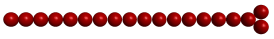
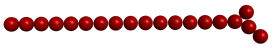
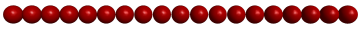
19M Energy: -24.33229396 	19N Energy: -23.38694748 	19O Energy: -23.27318493 
19P Energy: -22.30356055 		

SET IIb’

19Q Energy: -21.20826570 	19R Energy: -20.98809723 	19S Energy: -20.29574940 
19T Energy: -19.88718357 	19U Energy: -18.97362153 	19V -18.56341295 

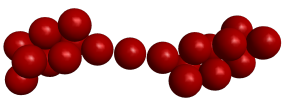
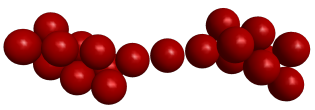
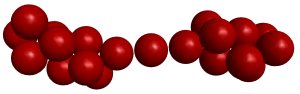
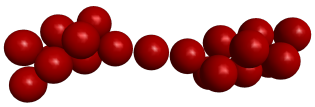
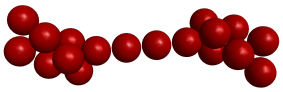
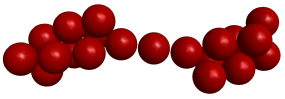
19W Energy: -16.78505999 		

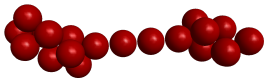
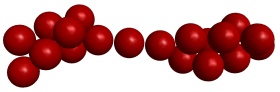
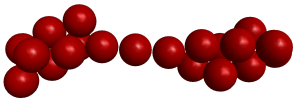
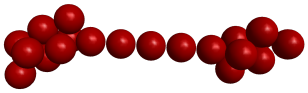
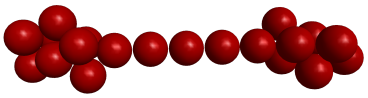
SET III

19X Energy: -11.10919223 	19Y Energy: -10.26071989 	19Z Energy: -9.87038493 
19ZA Energy: -9.34036978 		

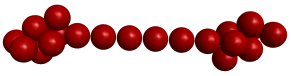
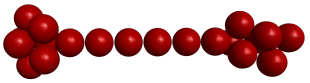
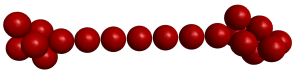
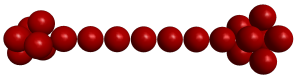
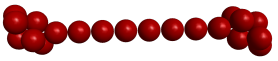
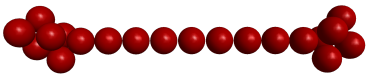
N=20

SET I

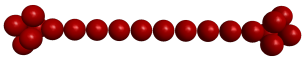
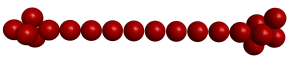
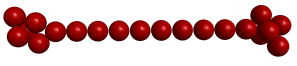
20A Energy:-27.29071051 	20B Energy: -27.29066707 	20C Energy: -27.11649813 
20D Energy: -27.10925345 	20E Energy: -27.04871448 	20F Energy: -27.04870115 

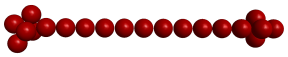
20G Energy: -26.99198881 	20H Energy: -26.98188154 	20I Energy: -26.98177700 
20J Energy: -26.47371152 	20K Energy: -26.29580256 	

SET IIa

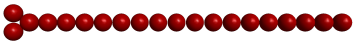
20L Energy: -25.77286678 	20M Energy: -25.73793923 	20N Energy: -24.83288862 
20O Energy: -24.80228231 	20P Energy: -23.86736332 	20Q Energy: -22.77417092 

SET IIb

20R Energy: -21.67470745 	20S Energy: -21.45411822 	20T Energy: -20.76142120 

20U Energy: -20.35164942 	20V Energy: -19.02713603 	

SET III

20W Energy: -11.57245490 	20X Energy: -10.72399393 	20Y Energy: -10.33364733 
20Z Energy: -9.80365022 		