

Low Temperature Behavior of the Lennard-Jones Polymer

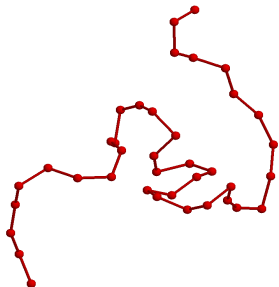
S.Schnabel

Institut für Theoretische Physik
Universität Leipzig

CompPhys 2008

the polymer

- off lattice
- 3 dimensions
- interaction between close monomers
- flexible bonds



interactions

$$E_{ij} = E_{LJ}(\min(r_{ij}, r_c)) - E_{LJ}(r_c)$$

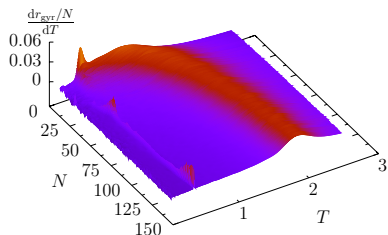
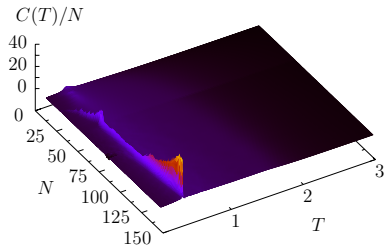
$$E_{LJ}(r) = 4[(\sigma/r)^{12} - (\sigma/r)^6]$$

$$E_{\text{FENE}}(r) = -\frac{K}{2}R^2 \ln(1 - [(r - r_0)/R]^2)$$

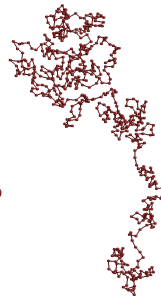
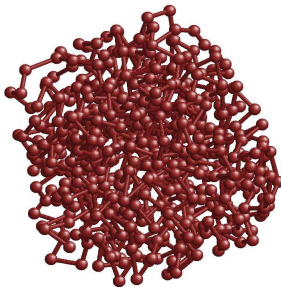
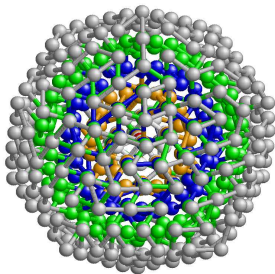
$$r_0 = 0.7 \quad \sigma = \frac{r_0}{2^{1/6}}$$

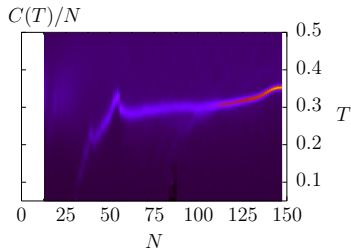
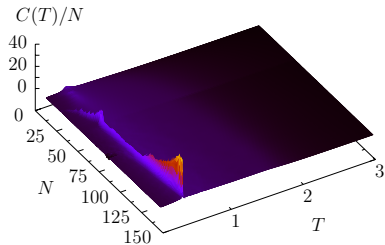
$$r_c = 2.5\sigma \quad K = 40 \quad R = 0.3$$

specific heat and fluctuation of radii of gyration

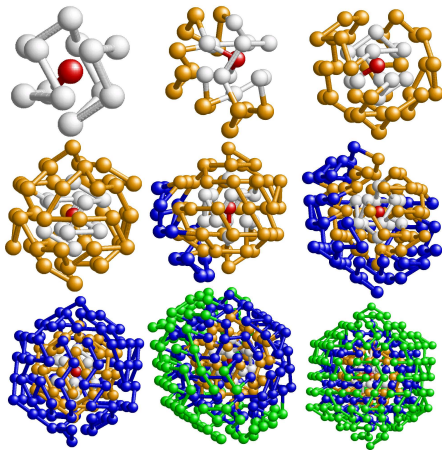


solid, globule and random conformation ($N = 561$)

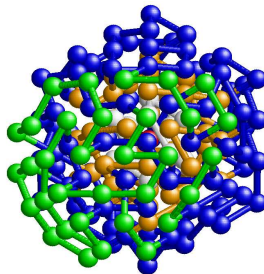
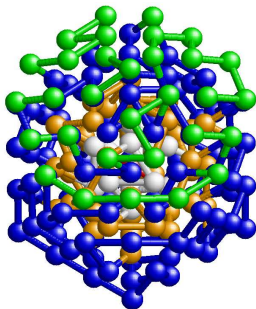


specific heat below $T = 0.5$ 

icosahedral conformations

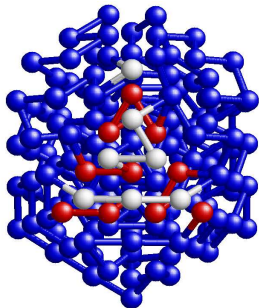


ground state conformations N=178,179

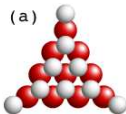


two different types of incomplete overlayer

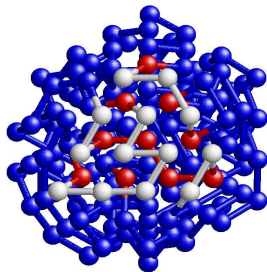
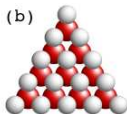
- hcp-like anti-Mackay (a)
- fcc-like Mackay (b)



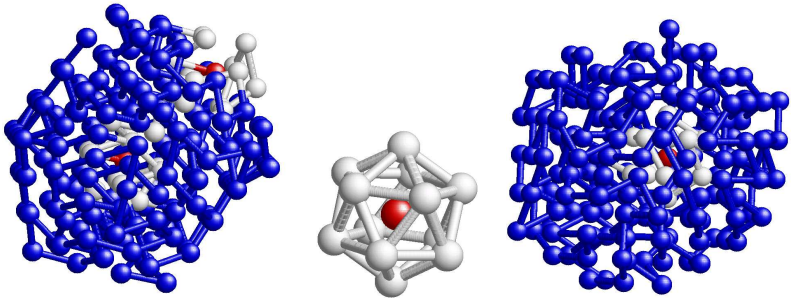
(a)



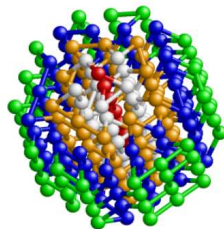
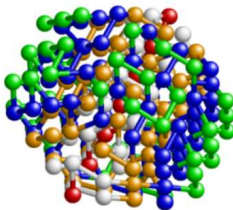
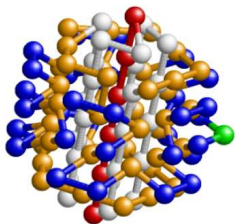
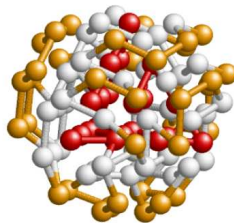
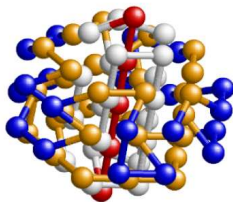
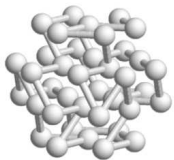
(b)



icosahedral cells



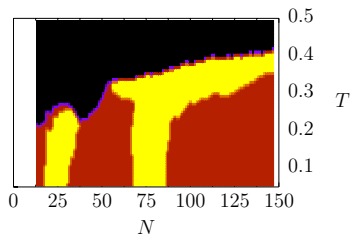
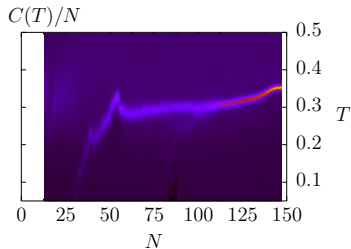
non-icosahedral energy minima

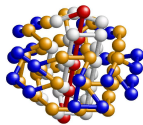
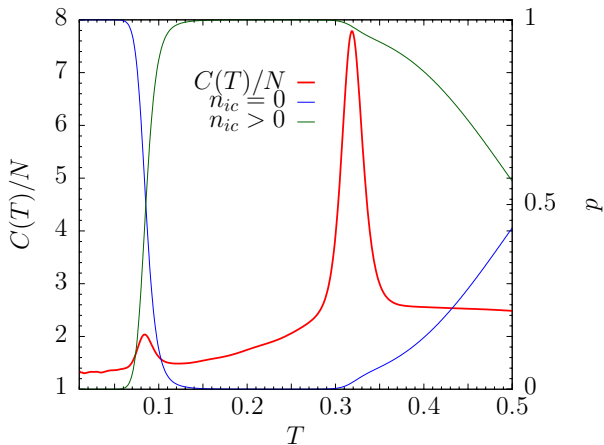


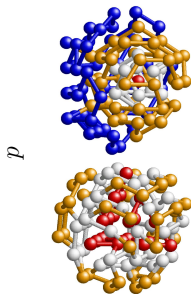
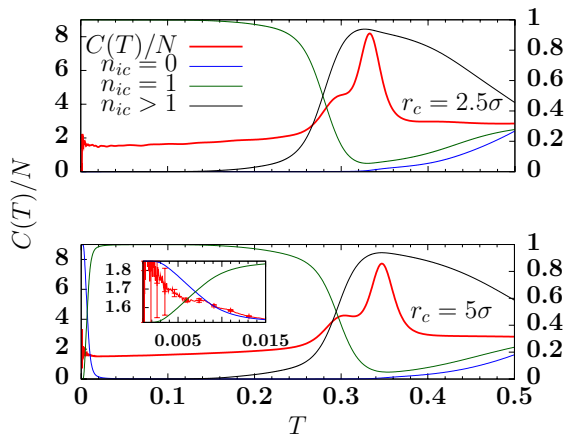
classification of a conformation's geometry (at small T)

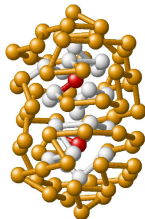
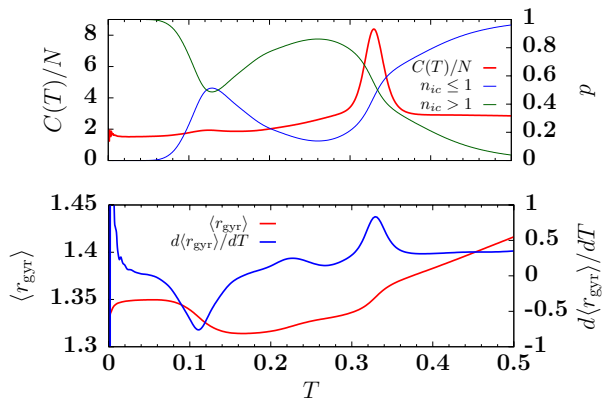
- no icosahedral cell : fcc, tetrahedral or decahedral
- one icosahedral cell : icosahedral (perhaps with incomplete Mackay overlayer or very few remaining monomers)
- two or more (incomplete) icosahedral cells : icosahedral with anti-Mackay overlayer

specific heat and structure below $T = 0.5$



thermodynamics $N = 75$ 

thermodynamics $N = 98$ $r_c = 2.5\sigma, 5\sigma$ 

thermodynamics $N = 87$ $r_c = 2.5\sigma$ 

summary

- broad similarities to Lennard-Jones clusters
- general Mackay anti-Mackay scheme holds also for polymers
- changing r_c might produce different ground states with new solid-solid transitions

Thanks for your attention