Self-Assembly of Linear polymer chains using spherically symmetric potentials.

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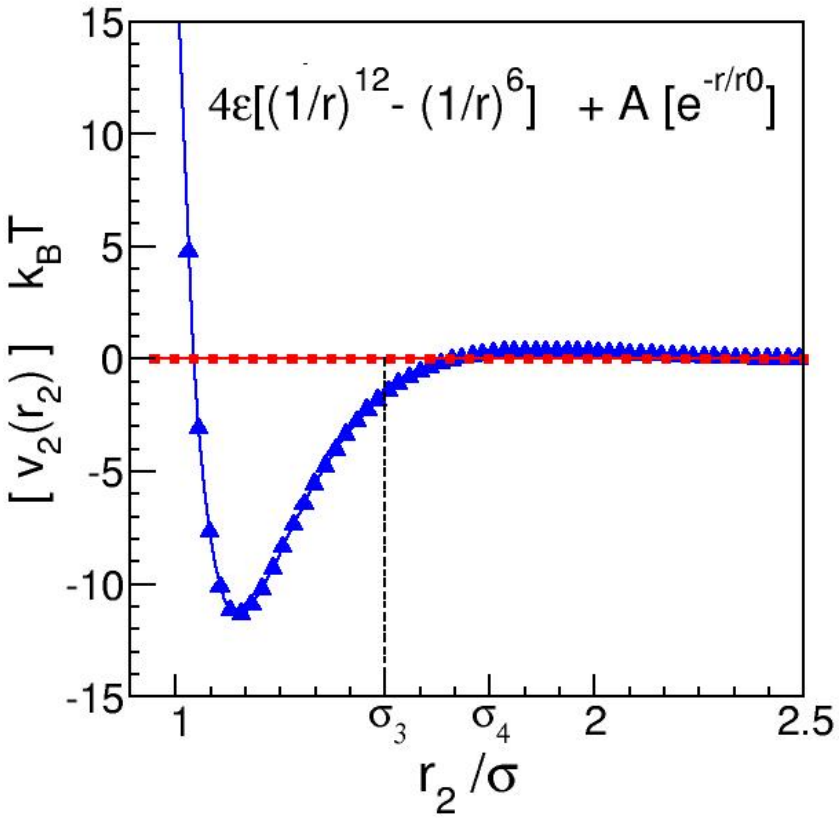
AIM: Model self-assembling polymer chains.

RAHUL PANDIT (1997)

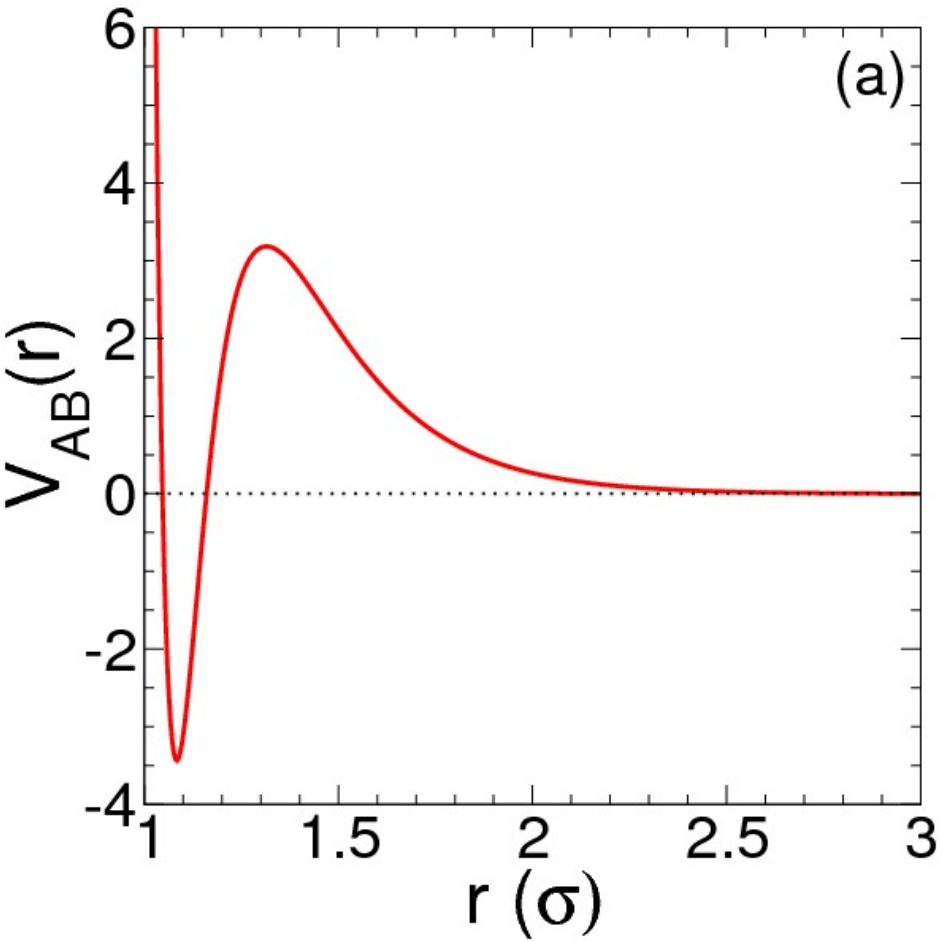
1. **Equilibrium/Living Polymers.**
2. **NO angle-dependent potentials V(r)**
3. **Semiflexible polymers: Micelles**
4. **No Branches.**



5. Self-assembly of Patchy colloids.
6. How to obtain **DIRECTED INTERACTIONS** starting out from spherically symmetric potentials ?

Phillip L. Geissler, ACS-Nano (2014):
Patterns without Patches: Hierarchical Self-Assembly of Complex Structures from Simple Building Blocks.

Used (24 – 12) potential with Screened Coulomb.



Potential :

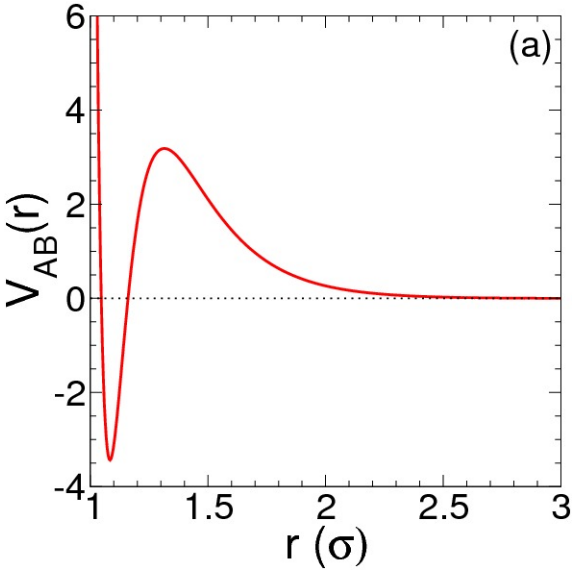
$$V_{AB}(r) = \epsilon_{AB}\left[\left(\frac{\sigma}{r}\right)^{24} - \left(\frac{\sigma}{r}\right)^{12}\right]$$

$$+ \epsilon_{AB}\left[\epsilon^{*}_{AB}\frac{e^{-(r/R_{AB})}}{r}\right], ..\forall r < r_C$$

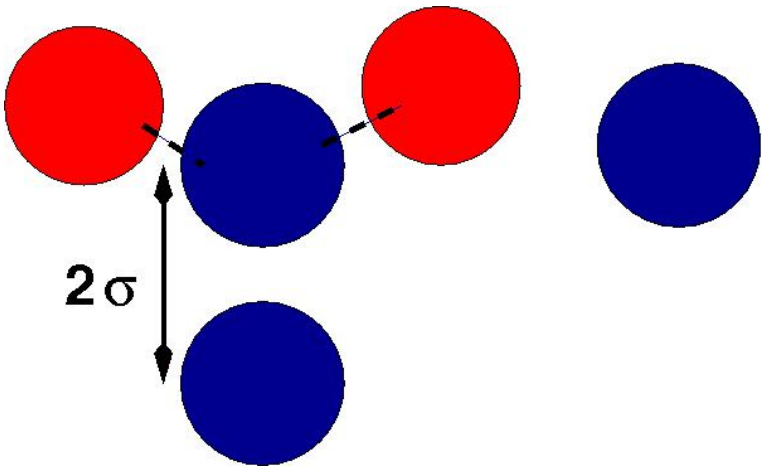
$\epsilon_{AB} = 105\, k_B\, T$, $\epsilon^{*}_{AB} = 16.81$,
$R_{AB} = 0.25\sigma$

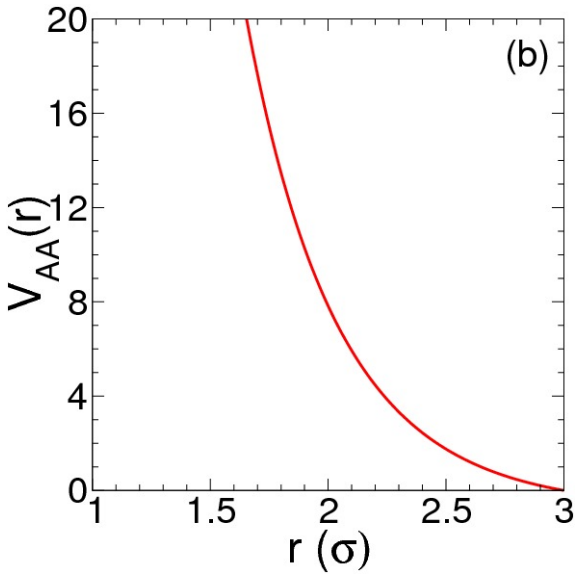
Polymeric Chains with branches.

Two kinds of particles: A and B: NO Branches.

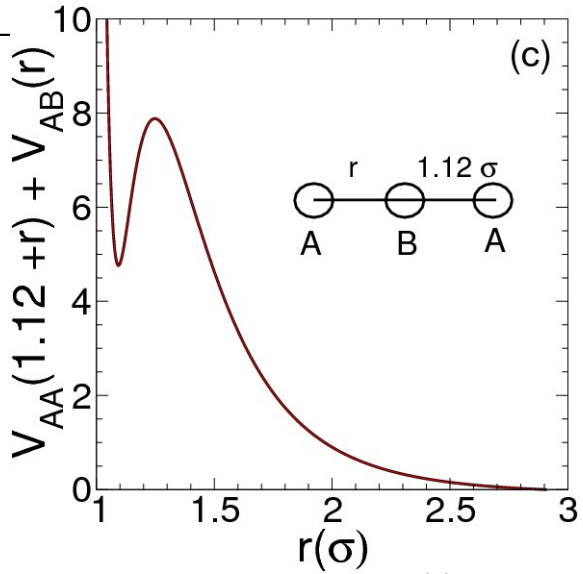


Between A-B particles.

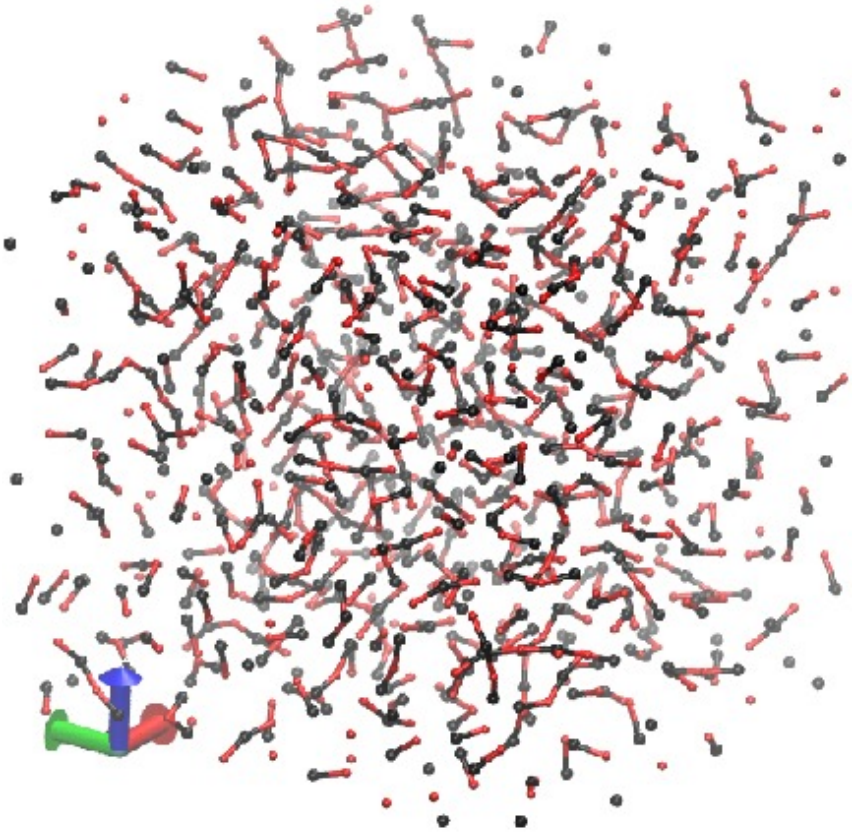




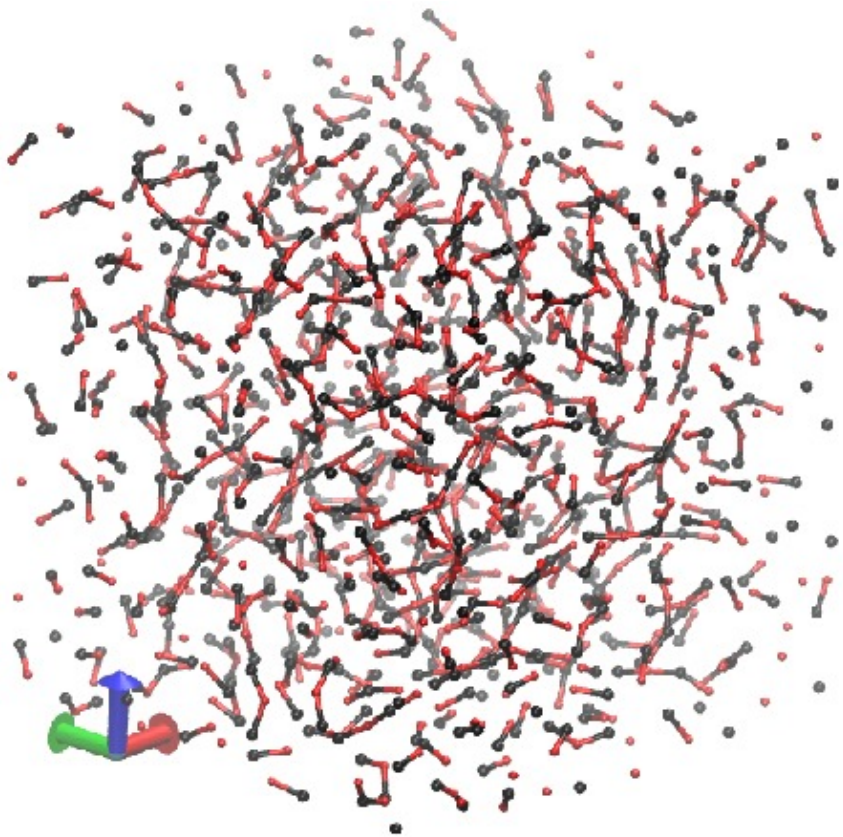
Repulsion: A-A OR B-B particles.



Self assembled Chains

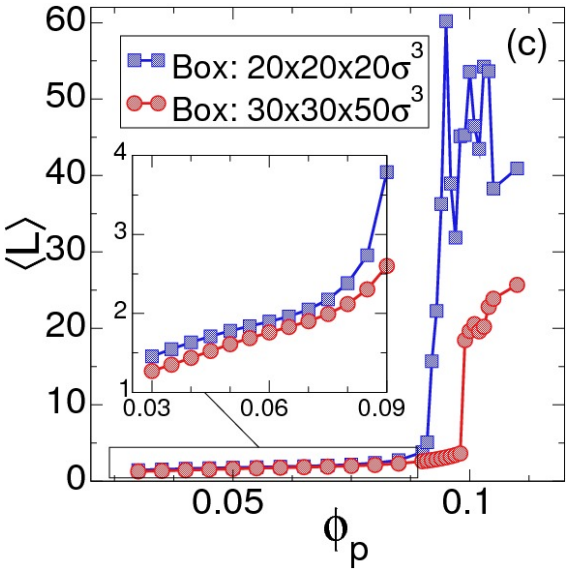


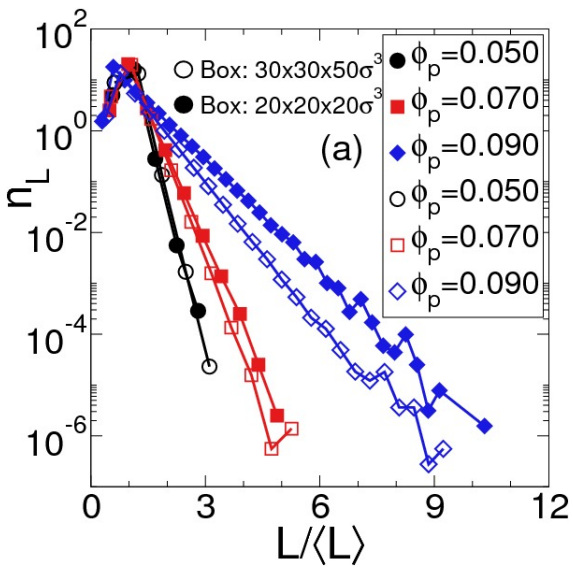
Number density $= \rho_m = 0.08\sigma^{-3}$.

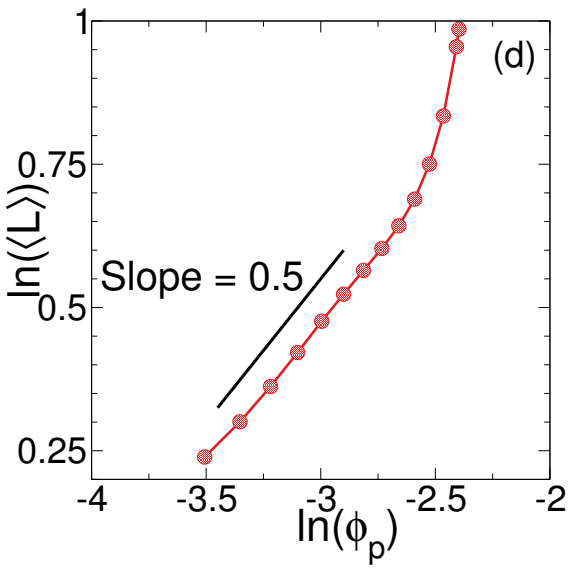


Number density $= \rho_m = 0.09\sigma^{-3}$.

Length Distributions

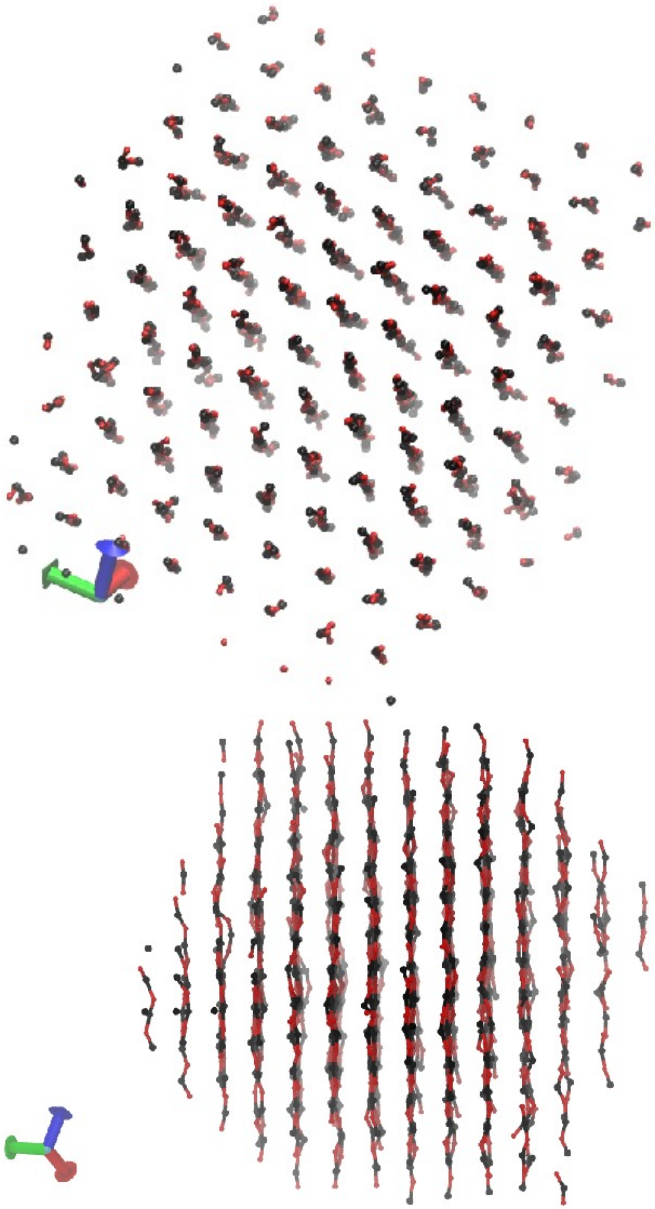


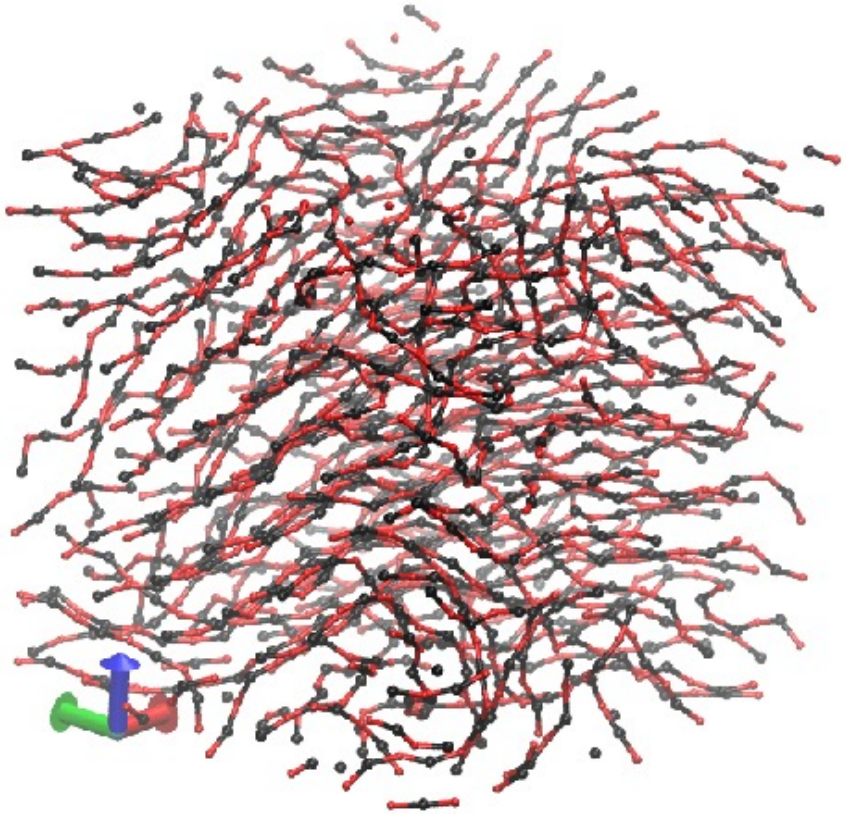




1. $< L >$ jumps as chains get line-hexgonal ordered.
2. Exponential distribution of lengths: Equilibrium polymers.
3. $< L > \sim \phi^{1/2}$ (volume fraction) [Cates and Candau-1991].

Further increase in Density:

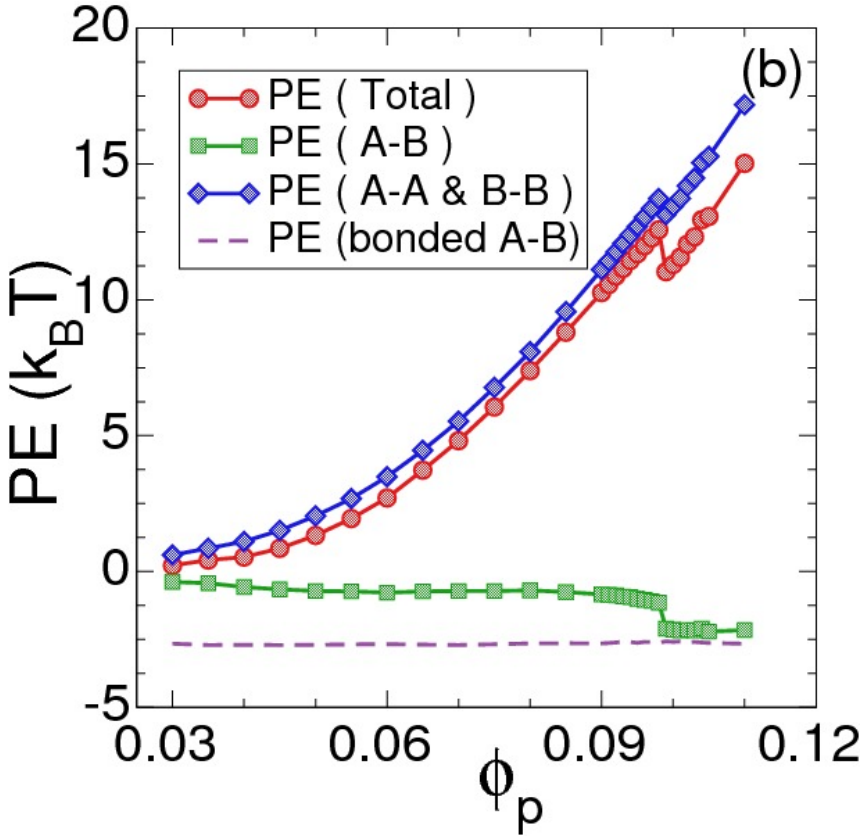


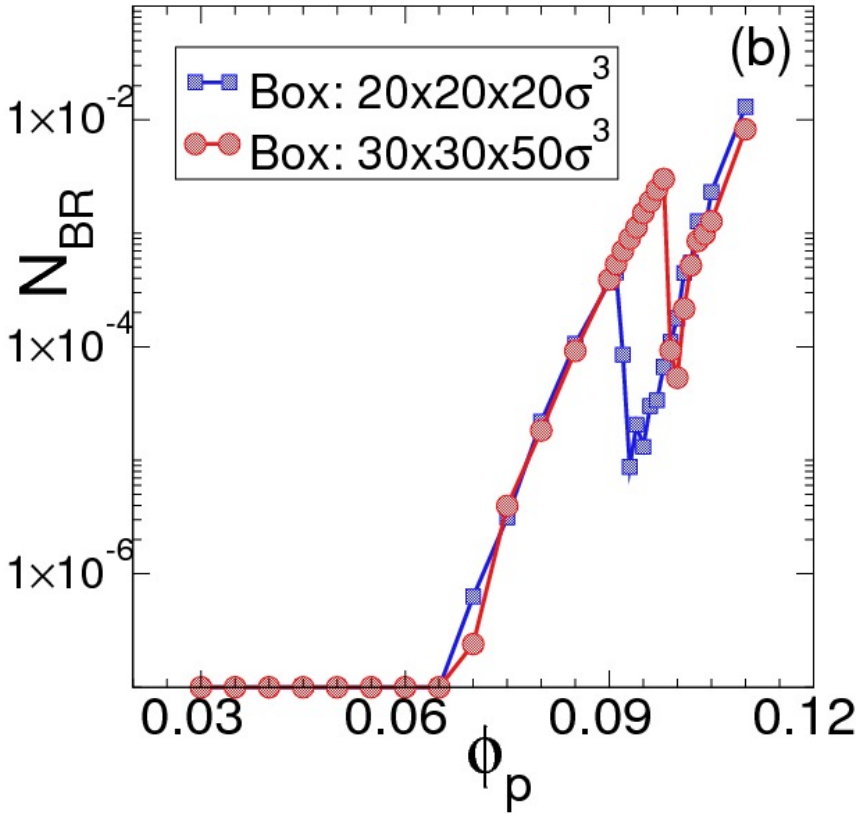


Gel with branches ($\rho_n = 0.12\sigma^{-3}$).

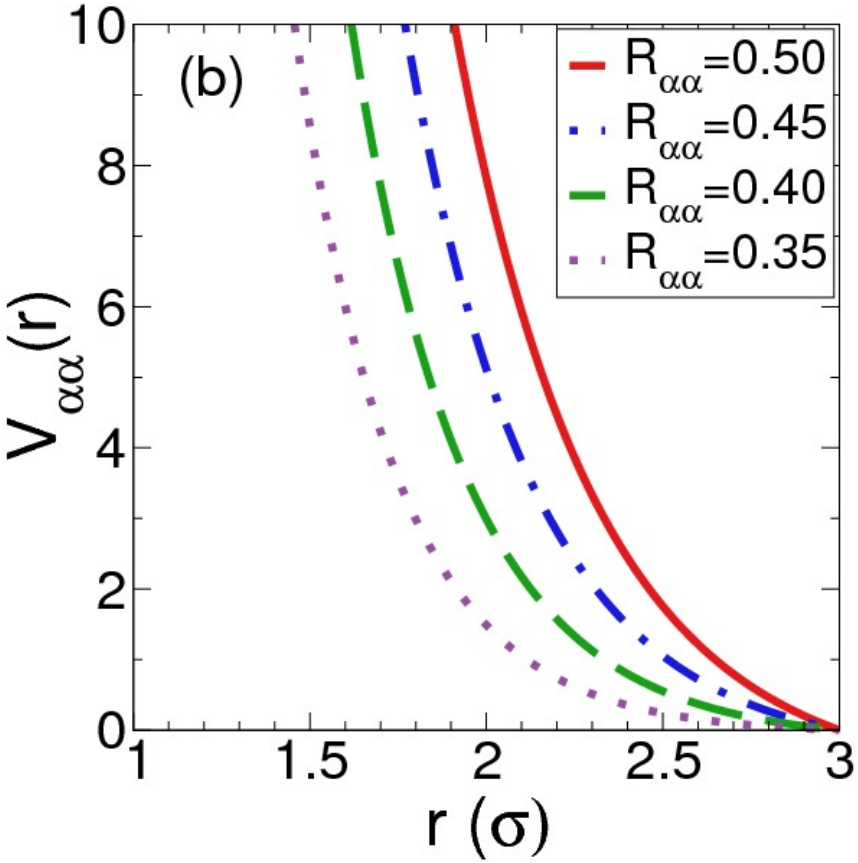
← **Line-Hexagonal** ($\rho_n = 0.095\sigma^{-3}$)

First Order transition to Line-hexagonal phase:

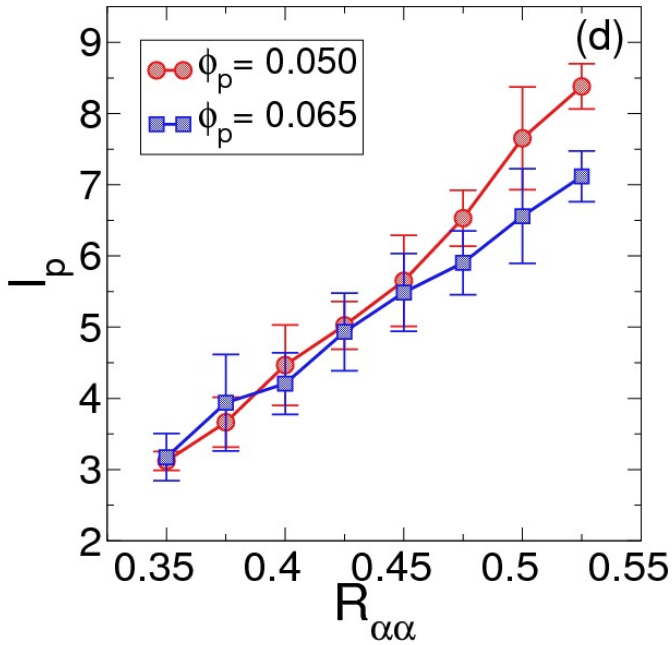


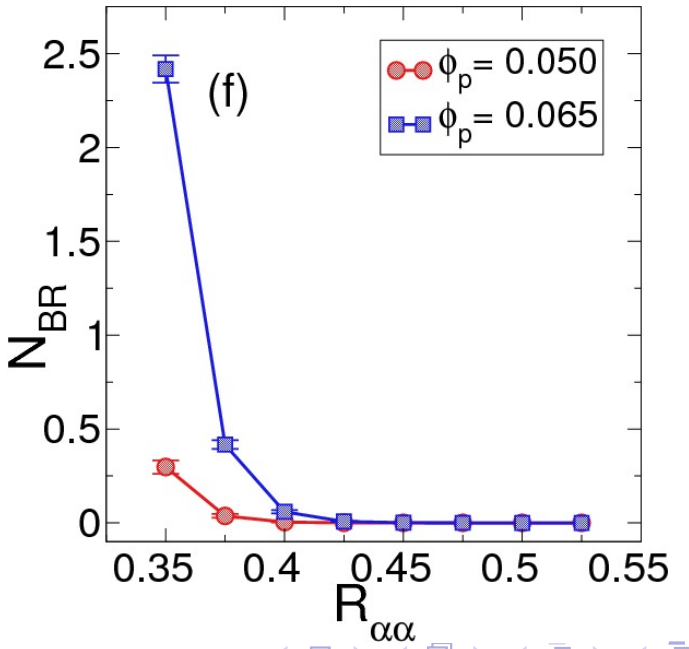


Tuneable persistence length l_p:



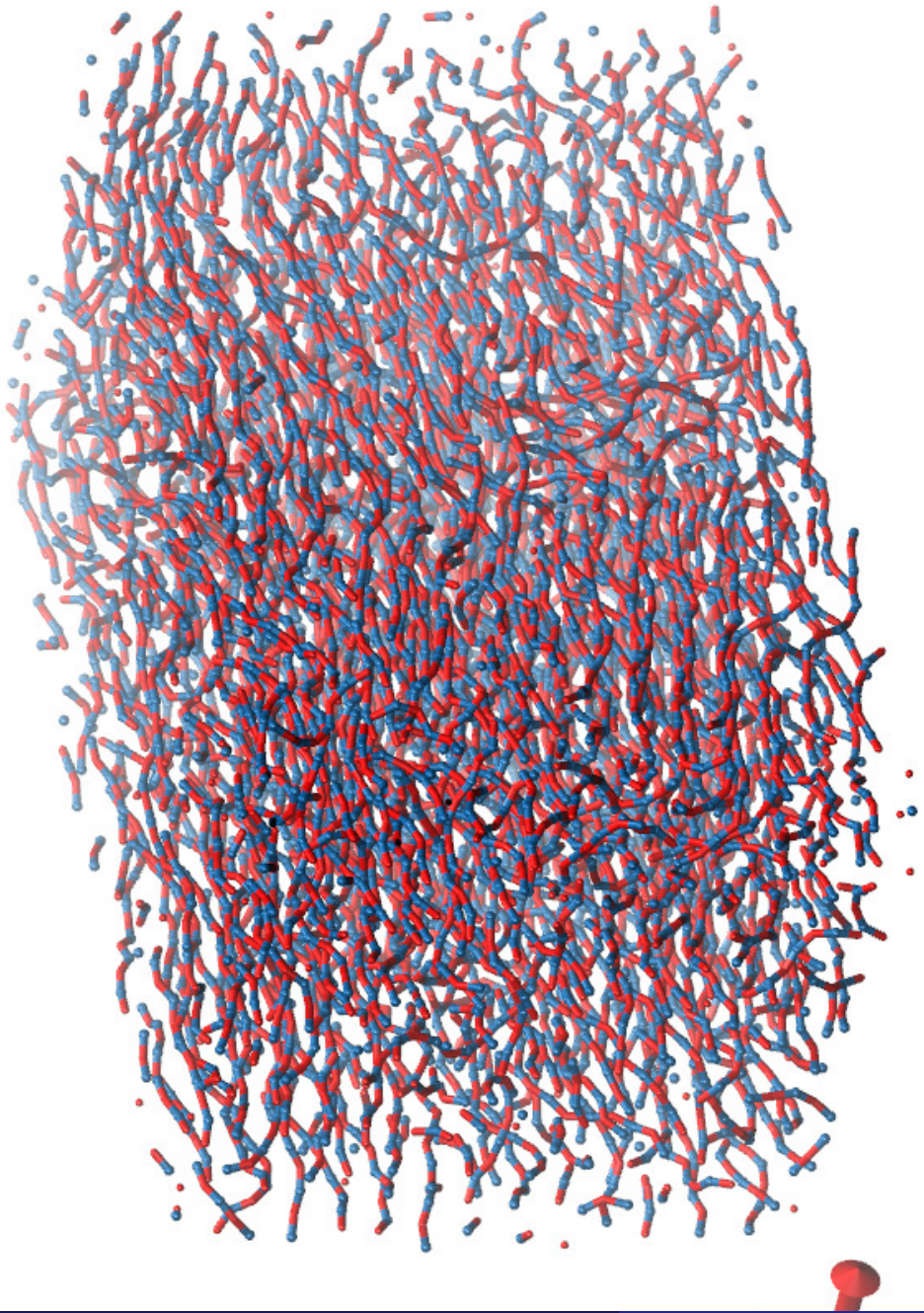
$V_{AA} = V_{BB} \sim e^{-r/R_{AA}}$

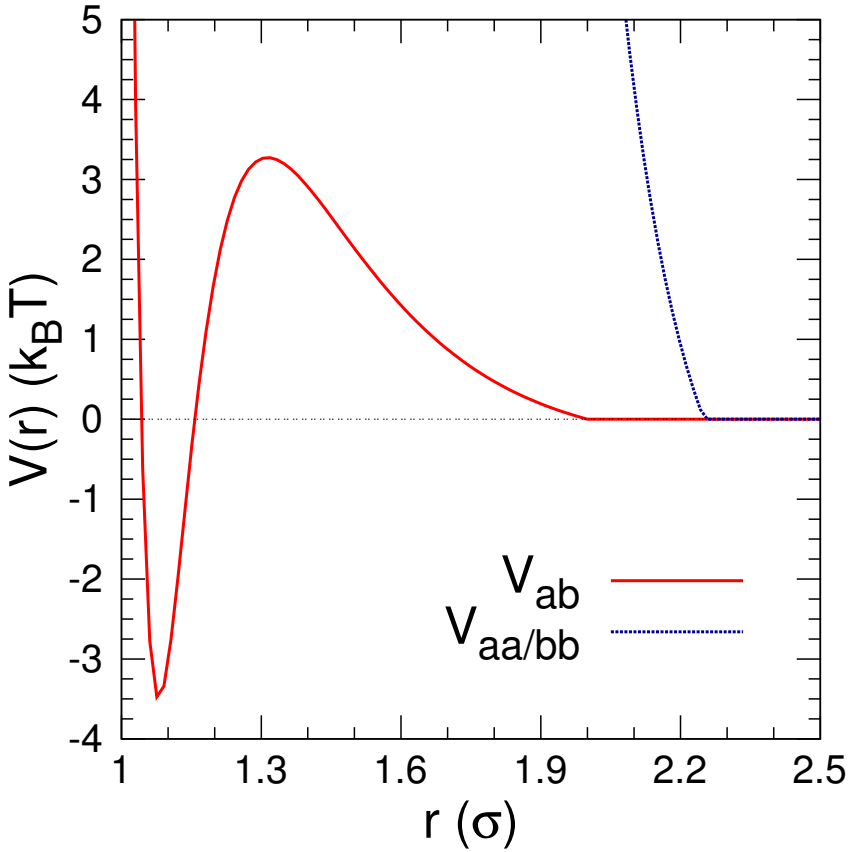




No. of branches $N_{BR} \rightarrow$

Nematic Phase





Conclusions

We obtain Self-assembled polymeric chains from specially designed spherically symmetric potentials with tuneable persistence length.

Alex Abraham.

ACKNOWLEDGEMENTS:

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https://arxiv.org/abs/1712.07154

THANK YOU.