

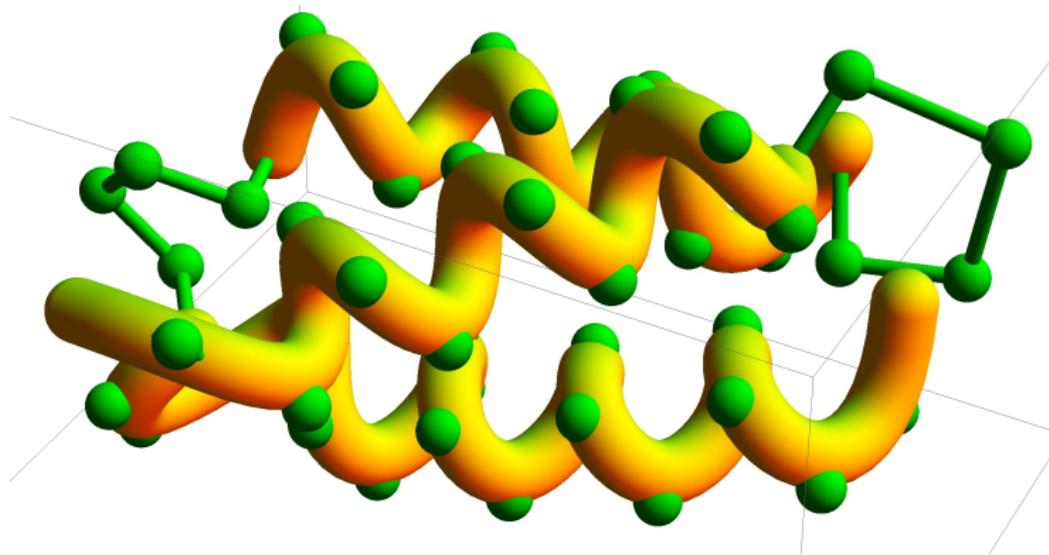
# Structure Formation In Helical Polymers

Matthew Williams and Michael Bachmann

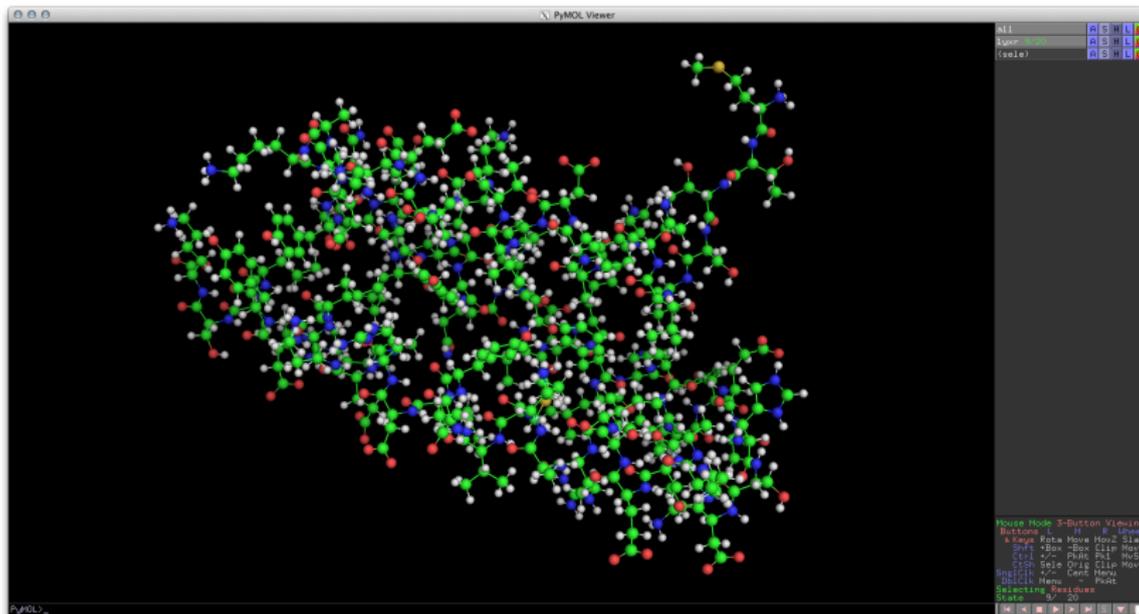
Soft Matter Systems Research Group

Center for Simulational Physics at The University of Georgia

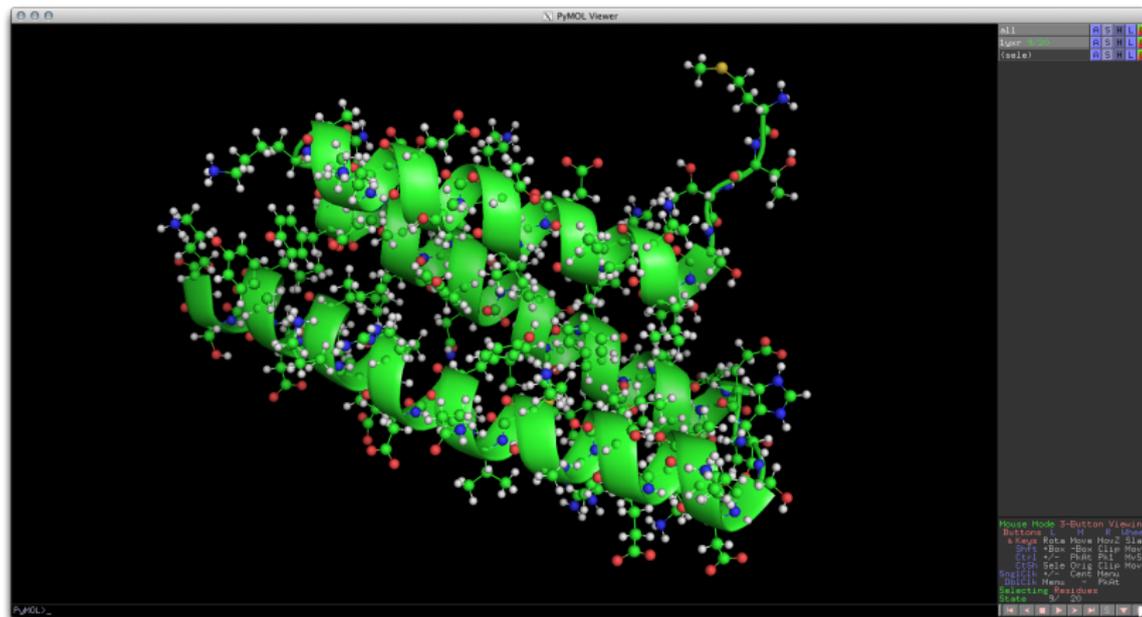
November 27, 2014



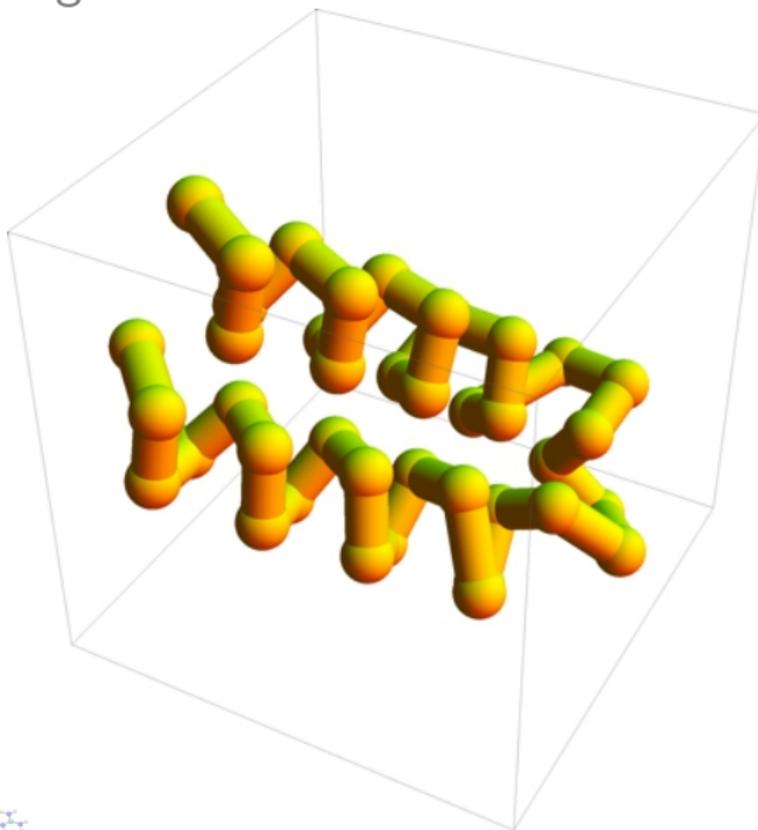
# Biopolymers



# Biopolymers



# Coarse Graining



# Model

- FENE Potential

Bonded interaction

$$U_{FENE} = -\frac{1}{2}KR^2 \log\left(1 - \left(\frac{r-r_0}{R}\right)^2\right)$$

- Lennard-Jones Potential

Non-bonded interaction

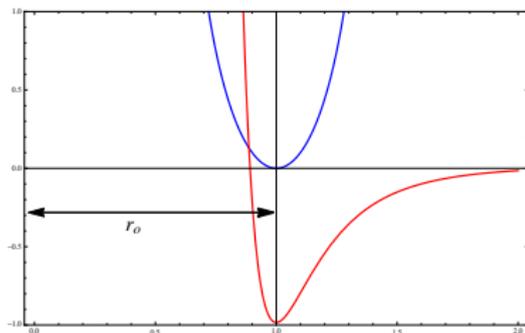
$$U_{LJ} = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$$

- Torsion Potential

$$E_\tau = S_\tau (1 - \cos(\tau - \tau_0))$$

- Bending Potential

$$E_\theta = S_\theta (1 - \cos(\theta - \theta_0))$$



D. C. Rapaport, PRE **66**, 011906 (2002)

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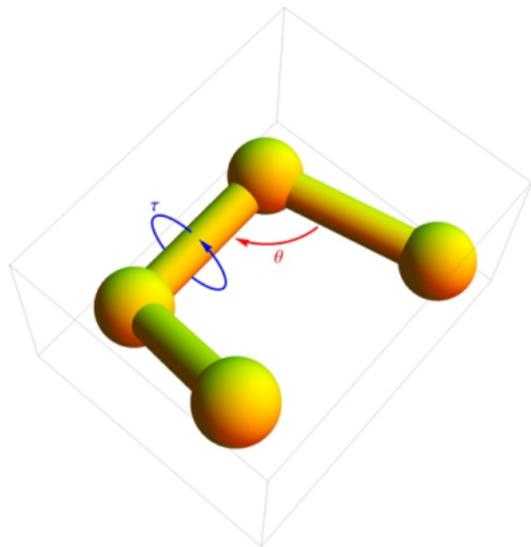
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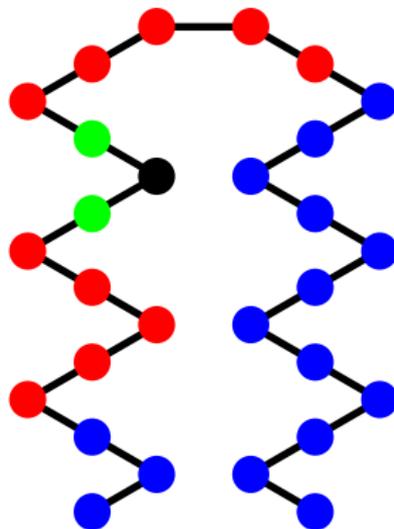
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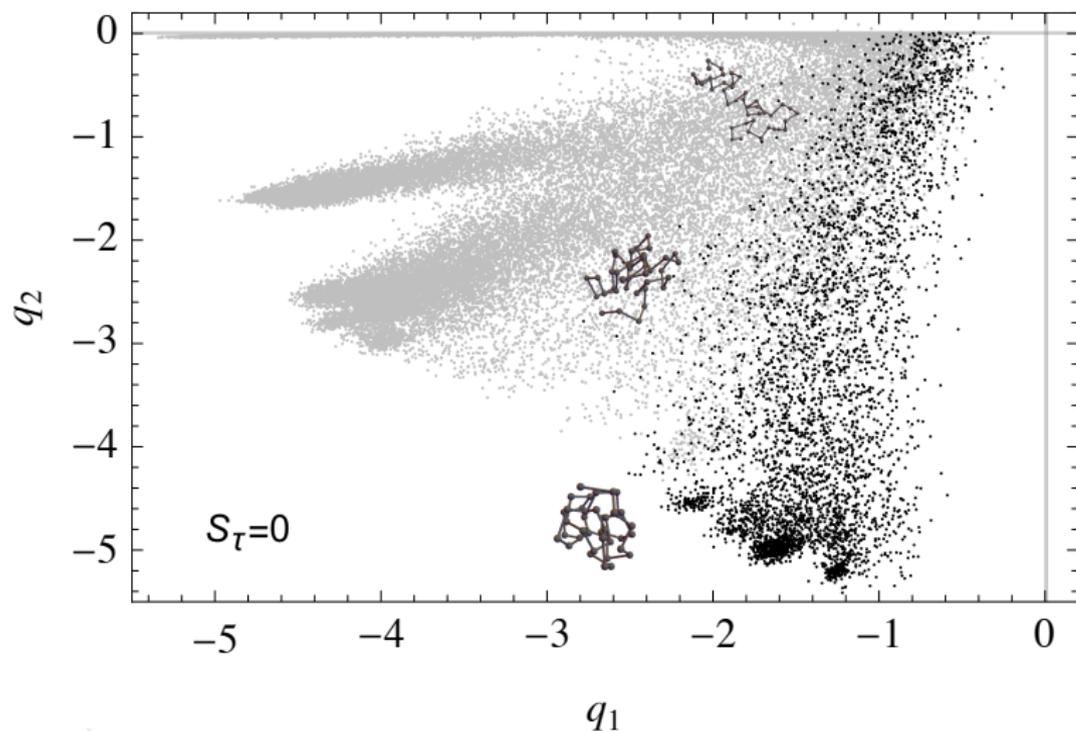
D. C. Rapaport, PRE **66**, 011906 (2002)

# Classification Parameters

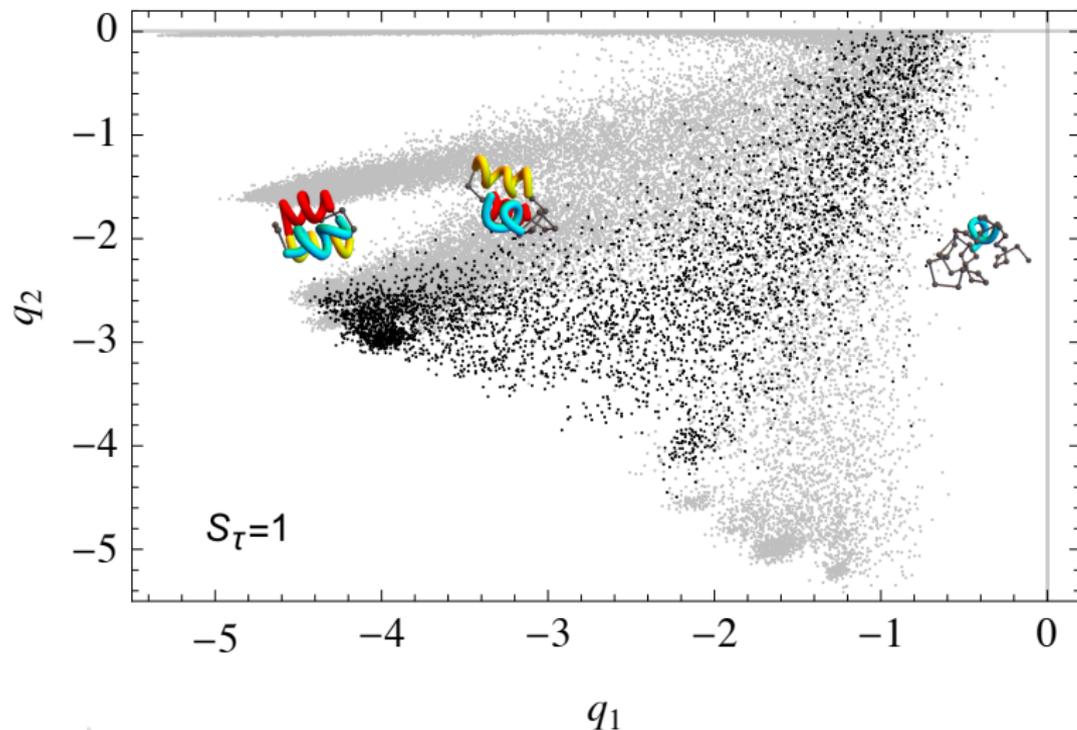
- Lennard-Jones Near ( $q_1$ )  
Interaction between monomers separated by less than or equal to 6 bonds  
(black with red)
- Lennard-Jones Far ( $q_2$ )  
Interaction between monomers separated by more than 6 bonds  
(black with blue)



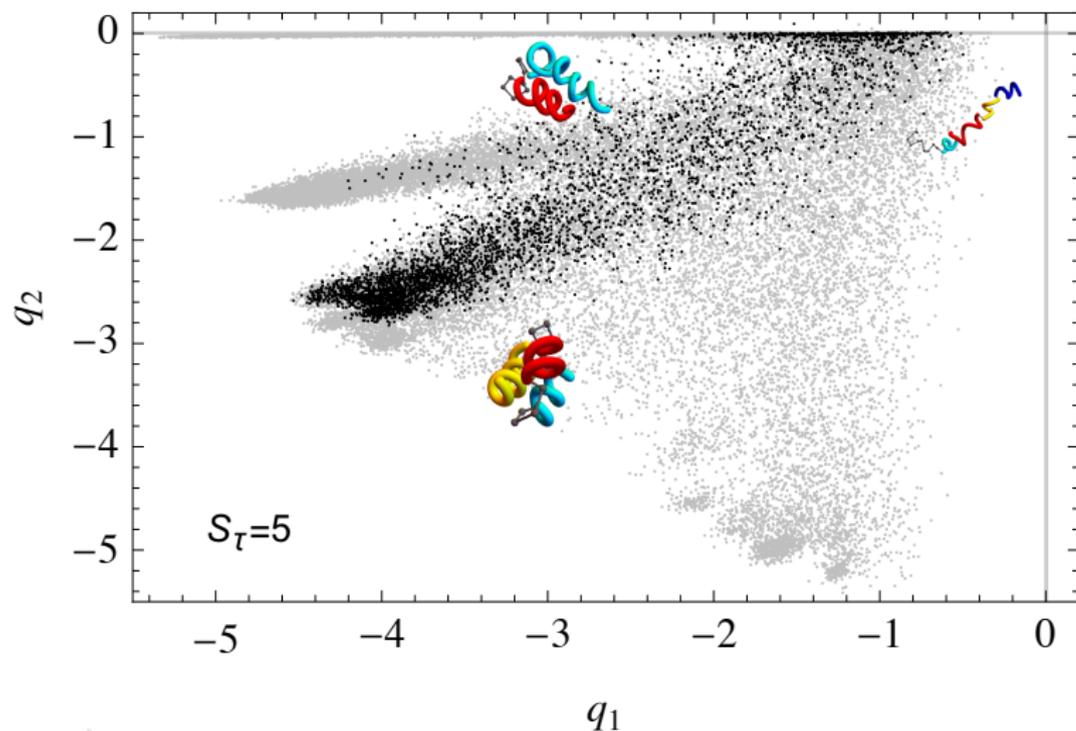
# 40 Monomers - Bending Restrained



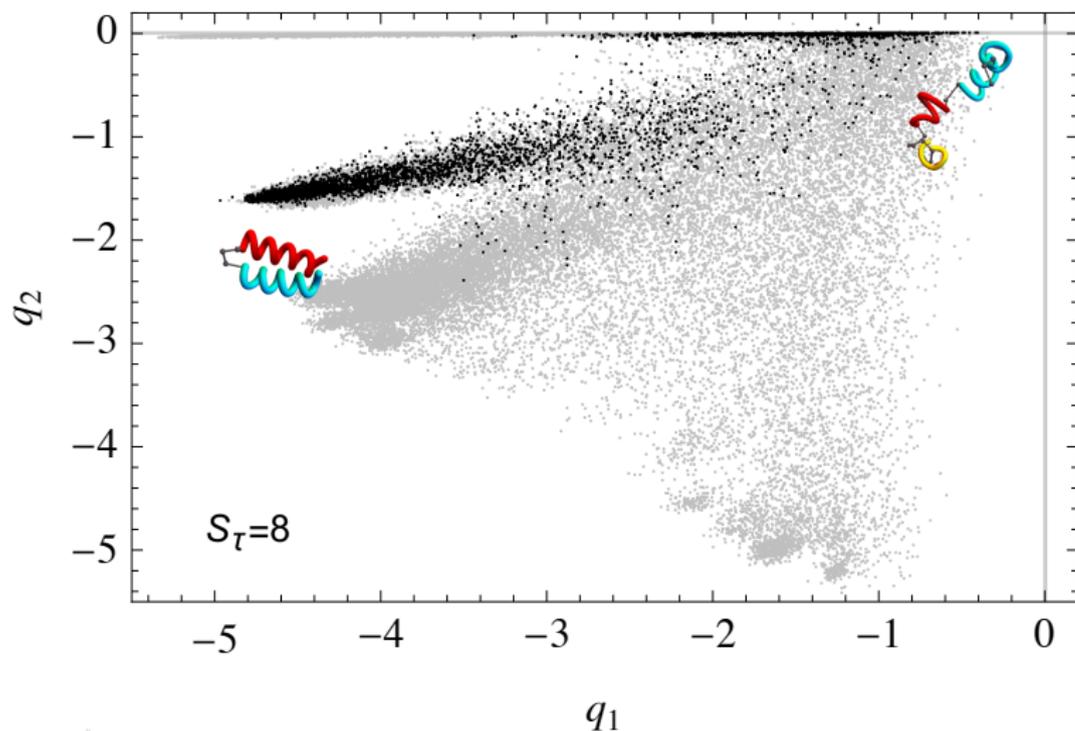
# 40 Monomers - Bending Restrained



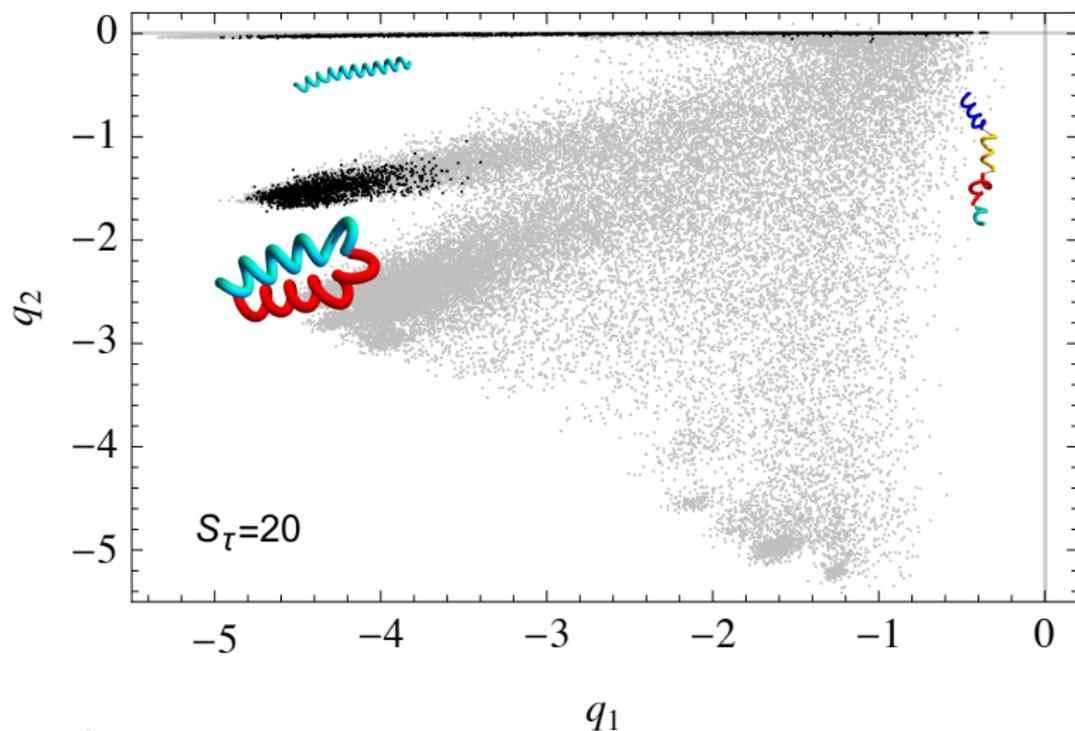
# 40 Monomers - Bending Restrained



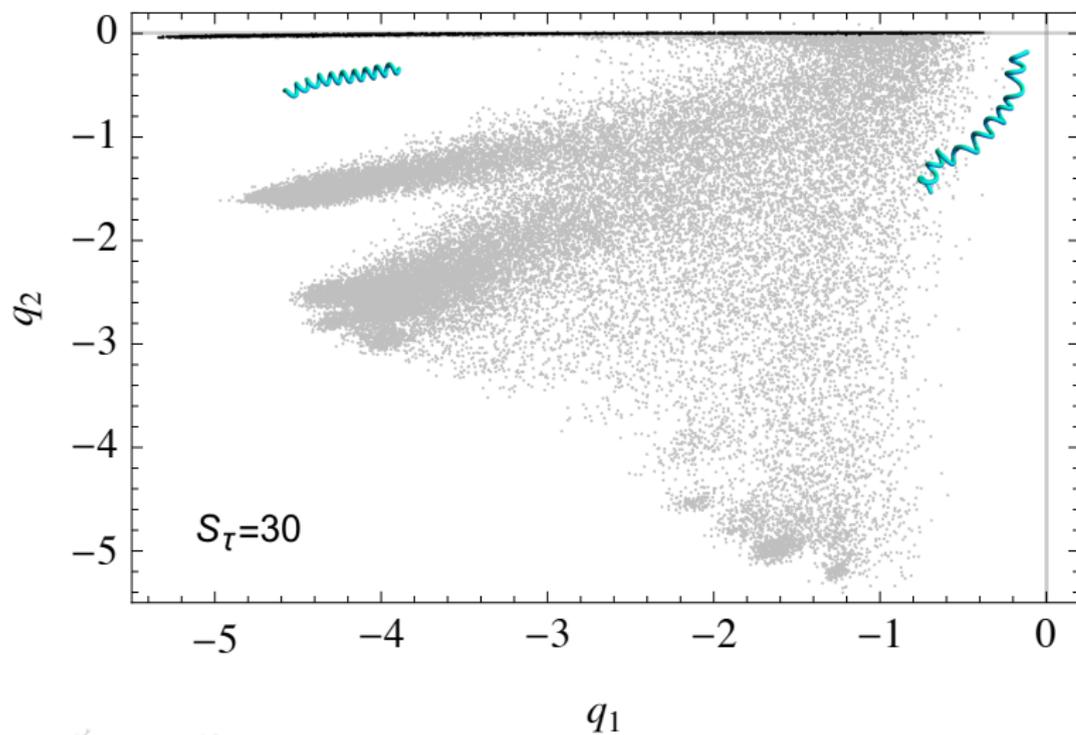
# 40 Monomers - Bending Restrained



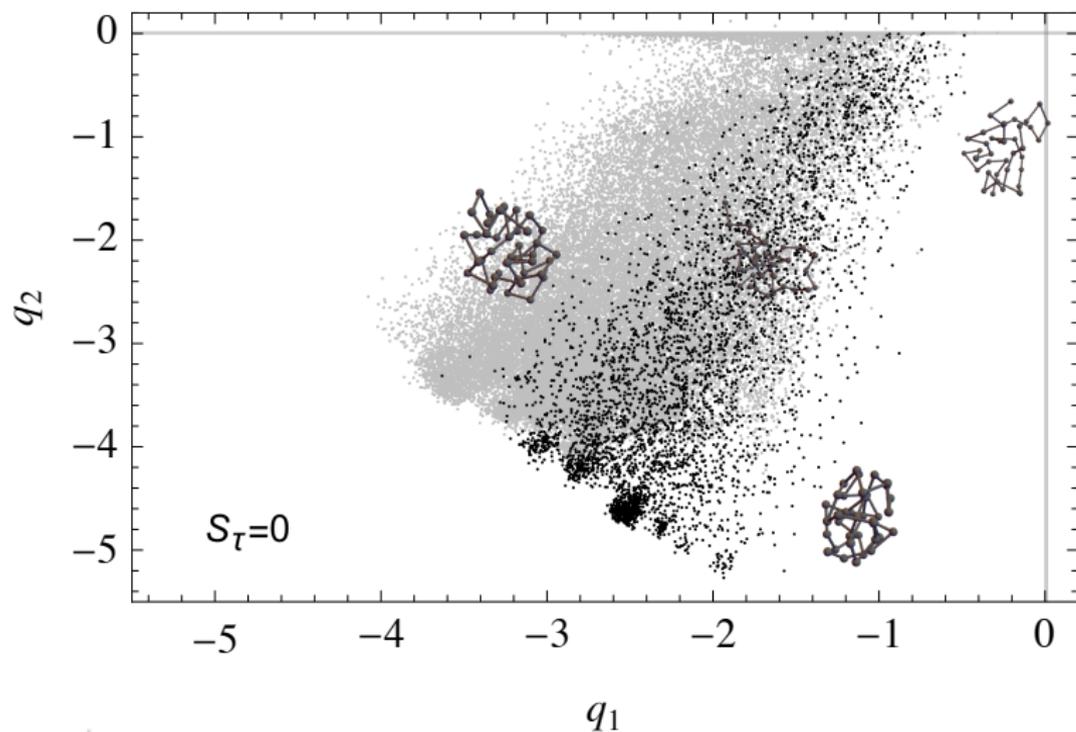
# 40 Monomers - Bending Restrained



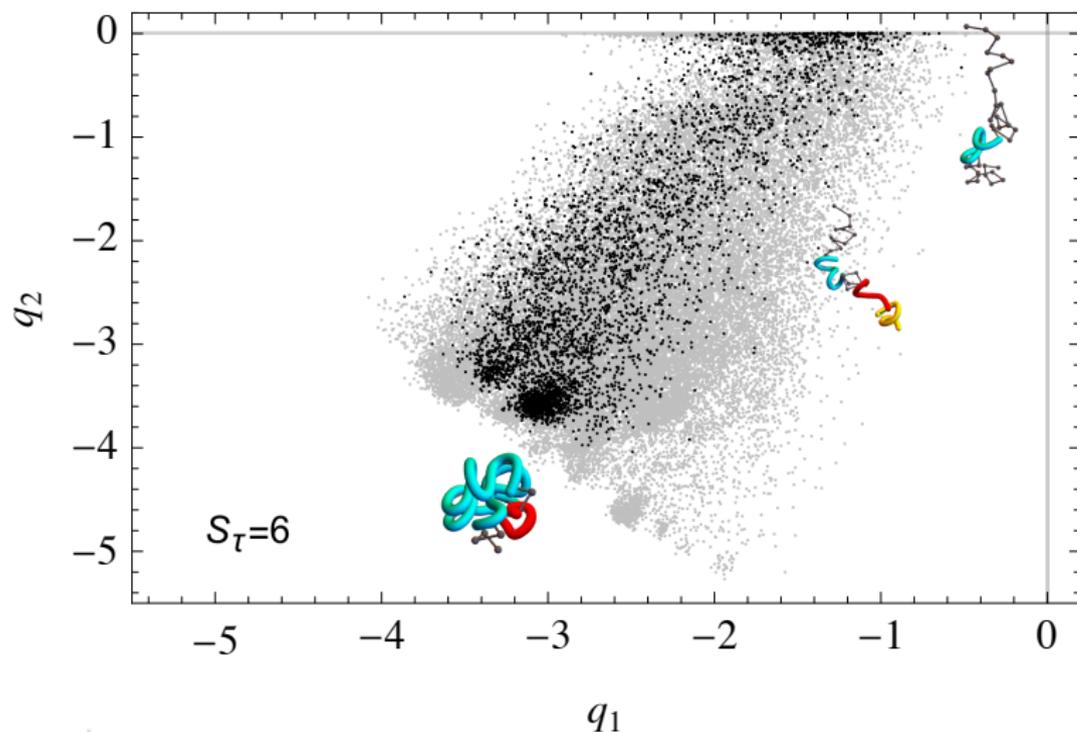
# 40 Monomers - Bending Restrained



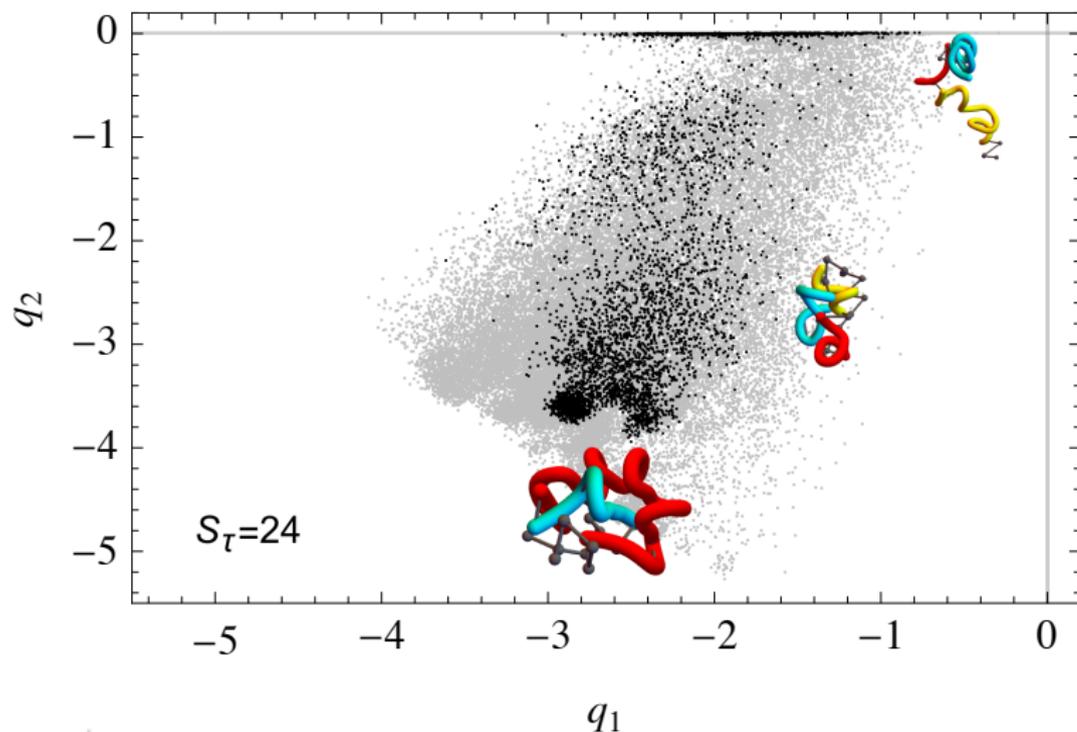
# 40 Monomers - Bending Unrestrained



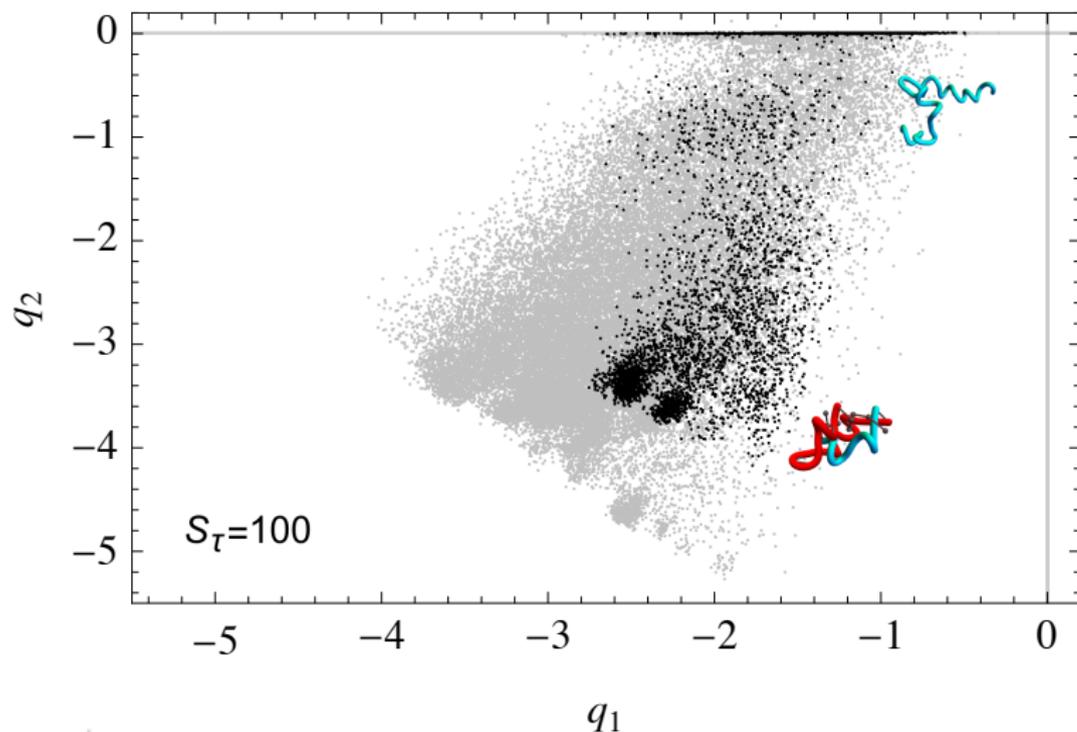
# 40 Monomers - Bending Unrestrained

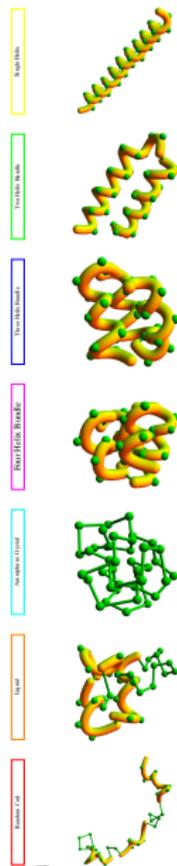
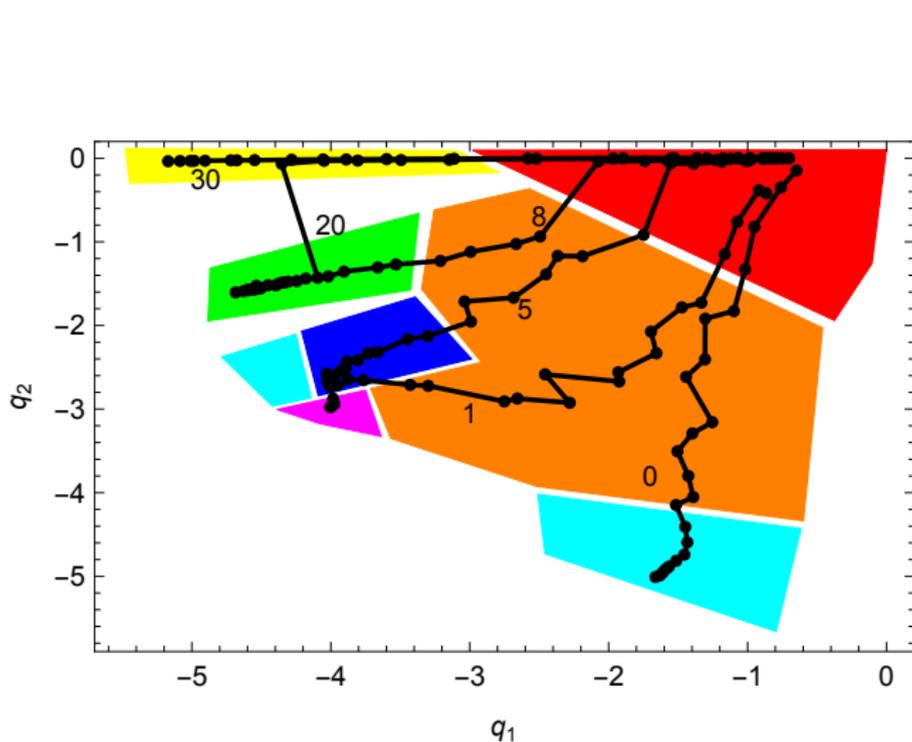


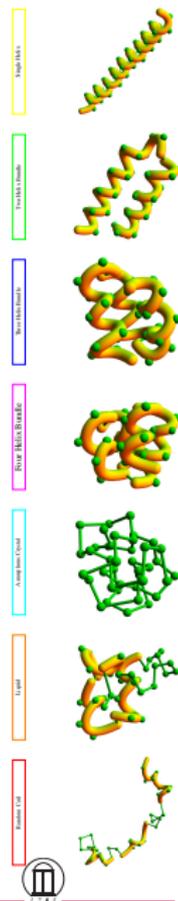
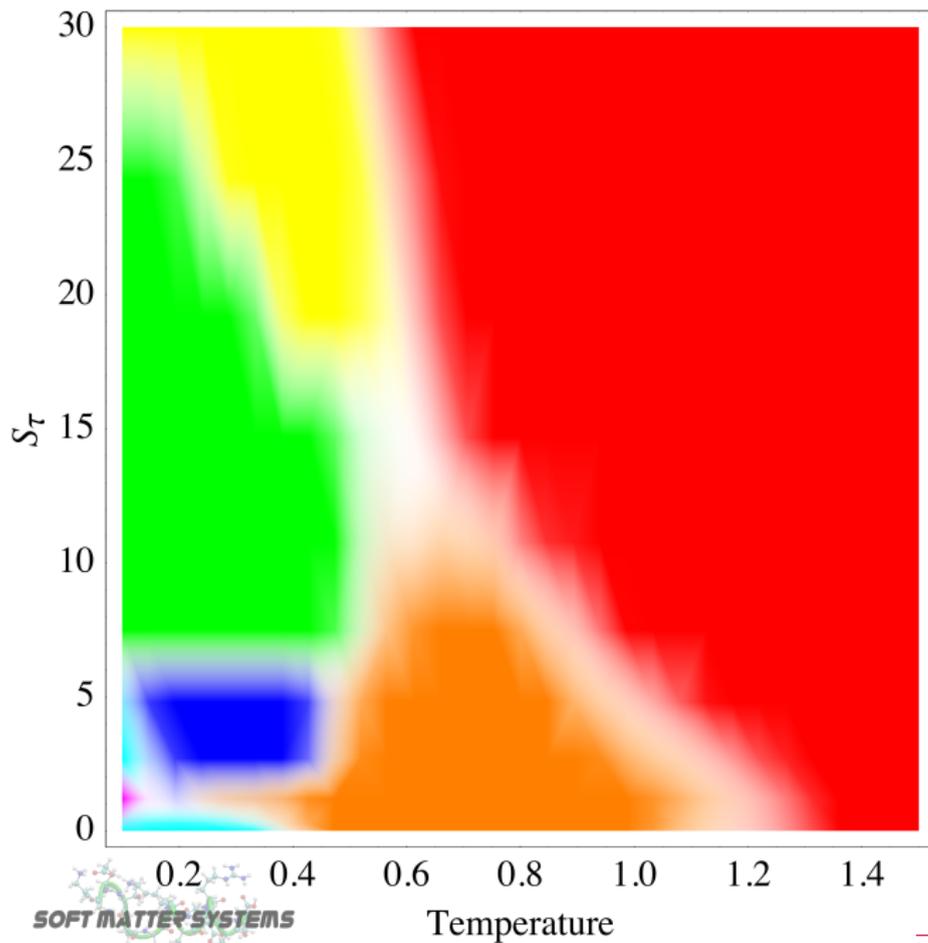
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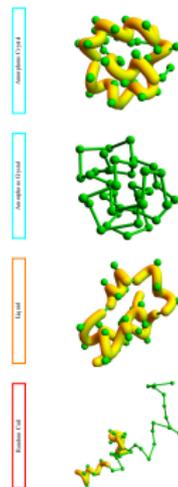
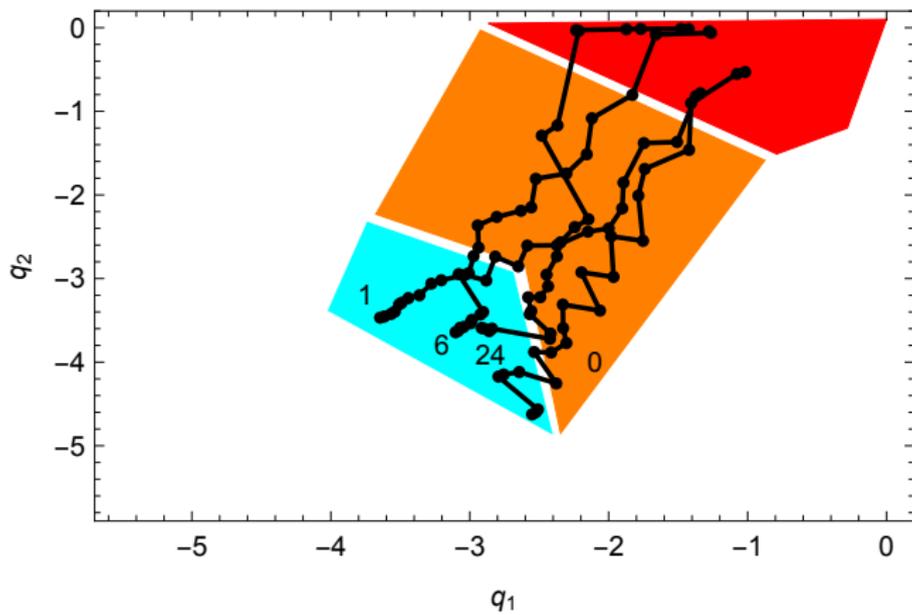


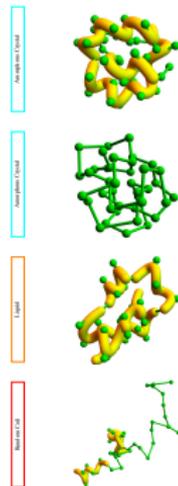
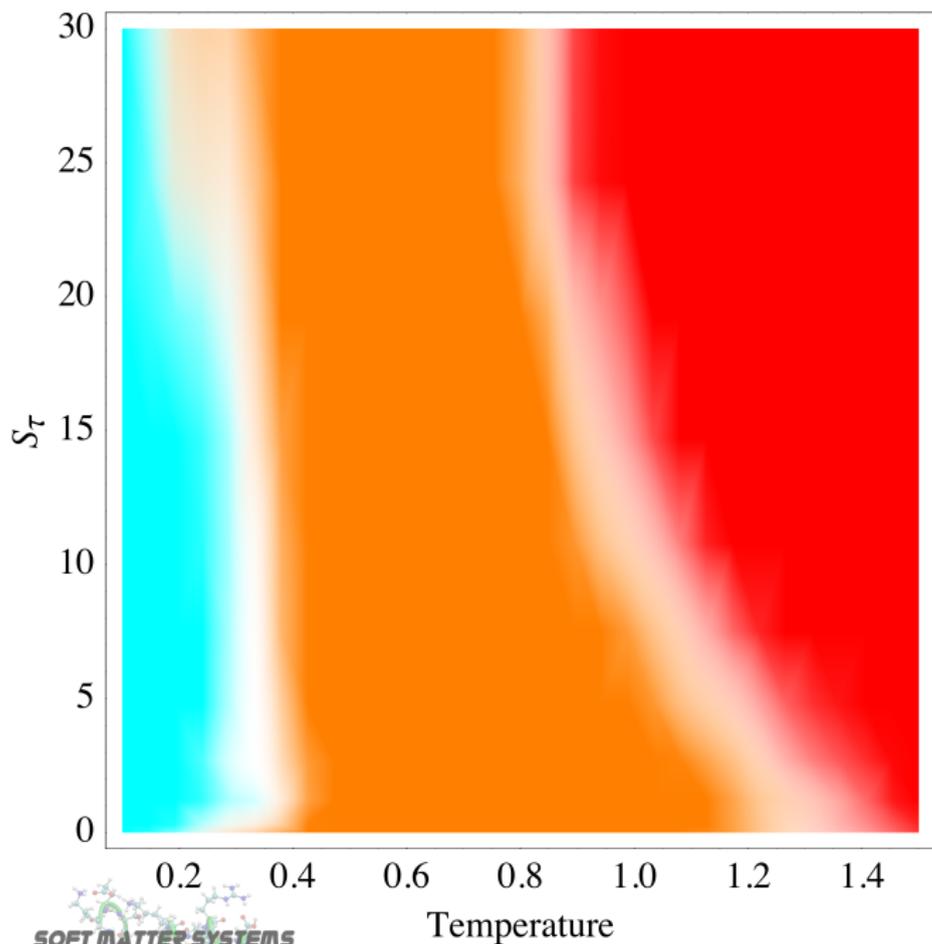
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# Conclusion

- Helical structures are dictated by a competition between the Lennard-Jones interaction and the torsion potential.
- Bending constraint acts to stabilize helical structures.
- Clustering of states space according to strategically chosen order parameters can be useful in picking out distinct phases.
- We are now exploring adsorption of helical polymers onto a substrate.

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