

# Double Interpenetrating Networks: Microphase Separation in Collapsed and Swollen States

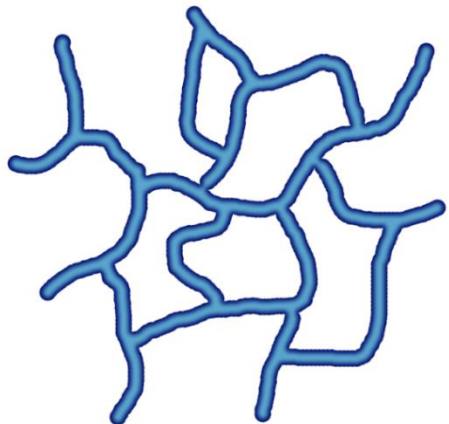
Alexander Chertovich

Alexei Gavrilov, Vladimir Rudyak, Pavel Kos and Elena Kozhunova

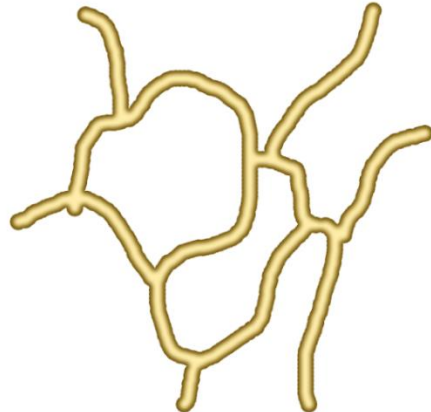
*Lomonosov Moscow State University*

# What is Double Interpenetrating Network?

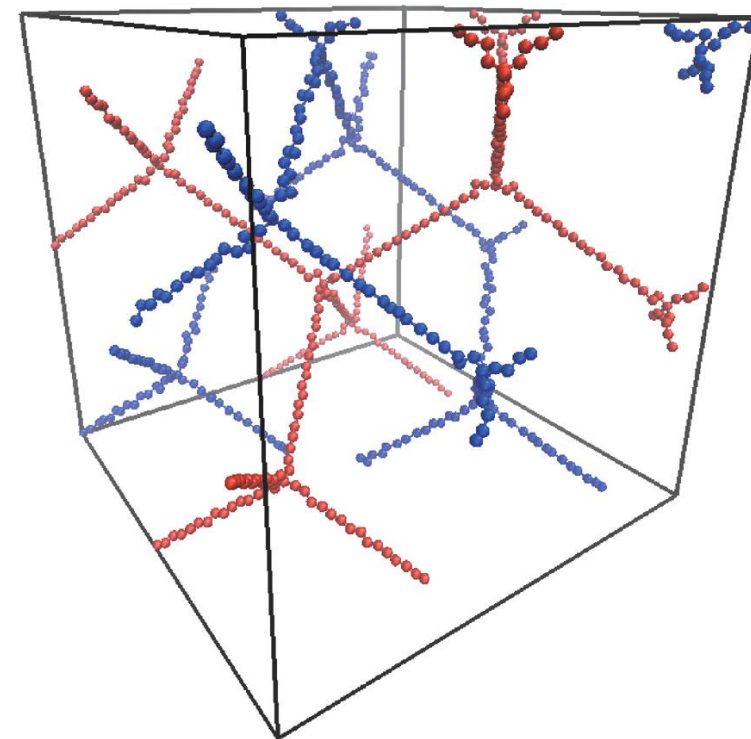
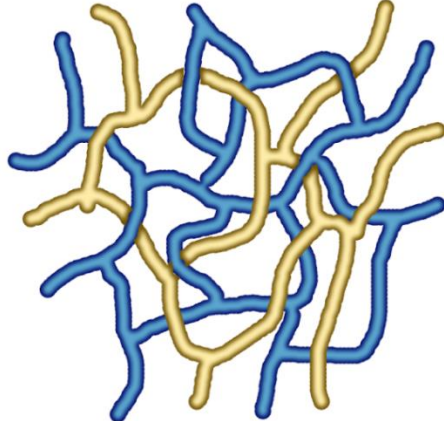
„A” network



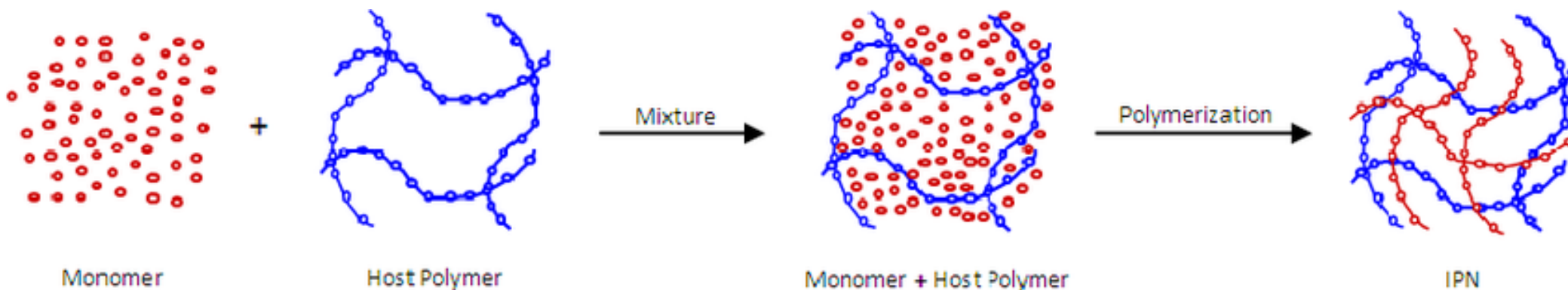
„B” network



IPN=„A”+„B”



Typical method of synthesizing:



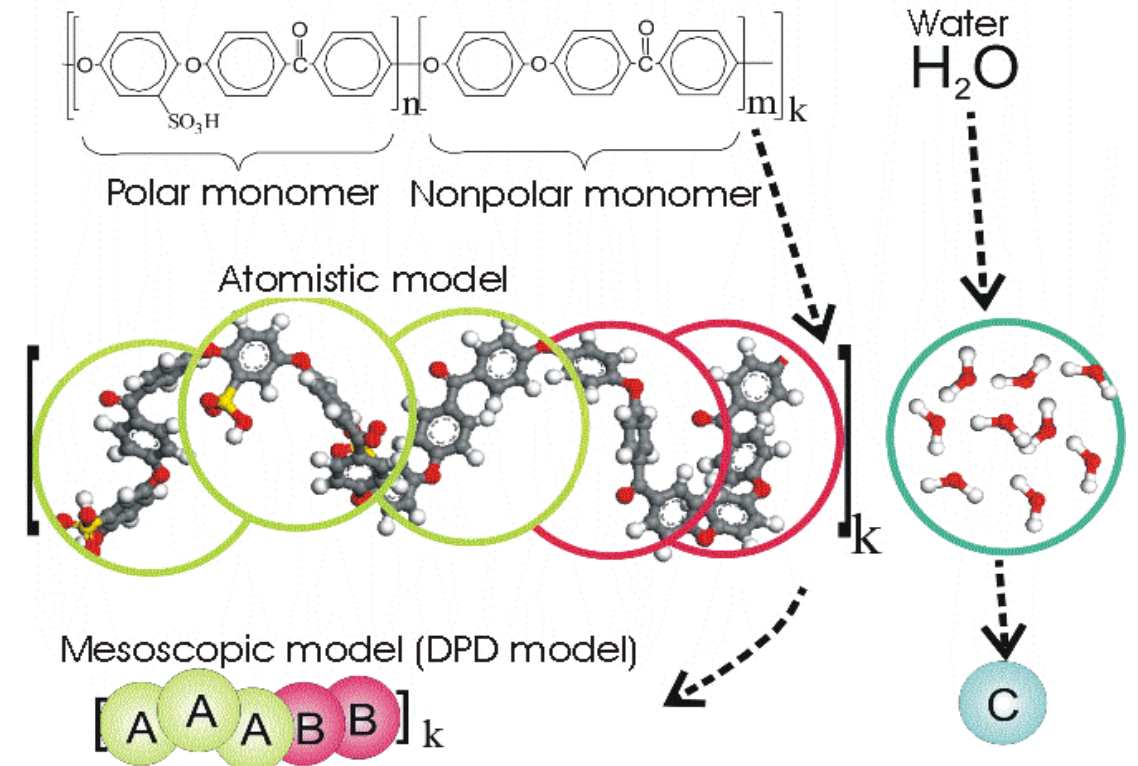
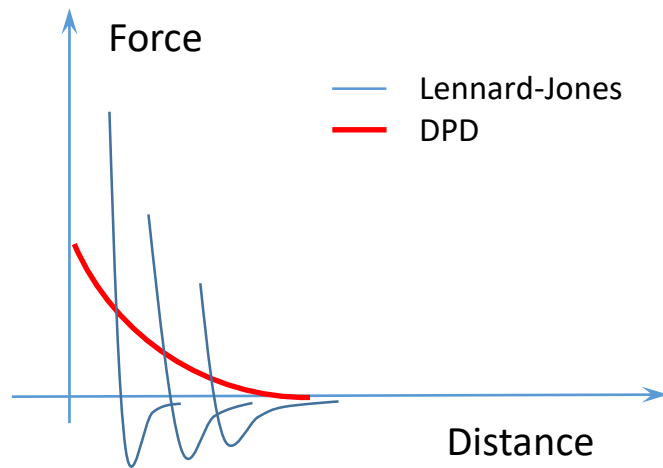
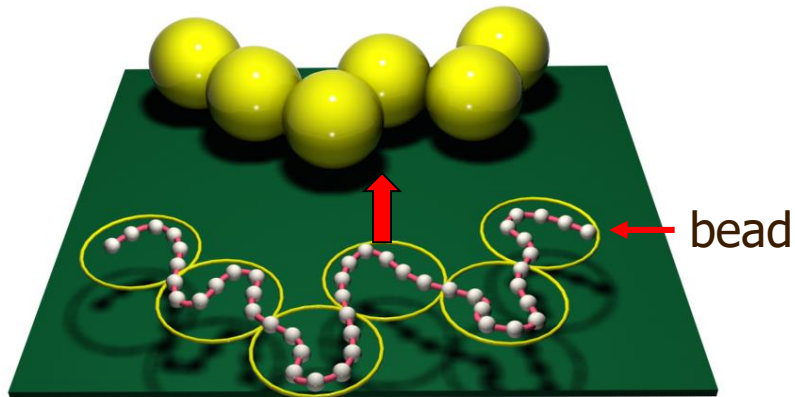
New class of polymer objects, which is not single molecule, but cannot be divided

# Computer simulation in soft matter and polymer science

DPD (Dissipative Particle Dynamics)

Groot R.D. and Warren P.B. *J. Chem. Phys.* **107** (1997) 4423

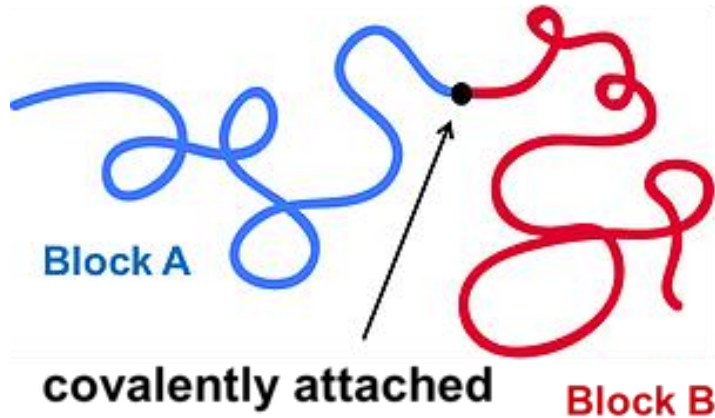
$$\mathbf{F}_{ij} = \mathbf{F}_{ij}^{Cons} + \mathbf{F}_{ij}^{Diss} + \mathbf{F}_{ij}^{Random}$$



Coarse-graining methodology allow to consider statistical physics (including conformational entropy) for very complex polymer system

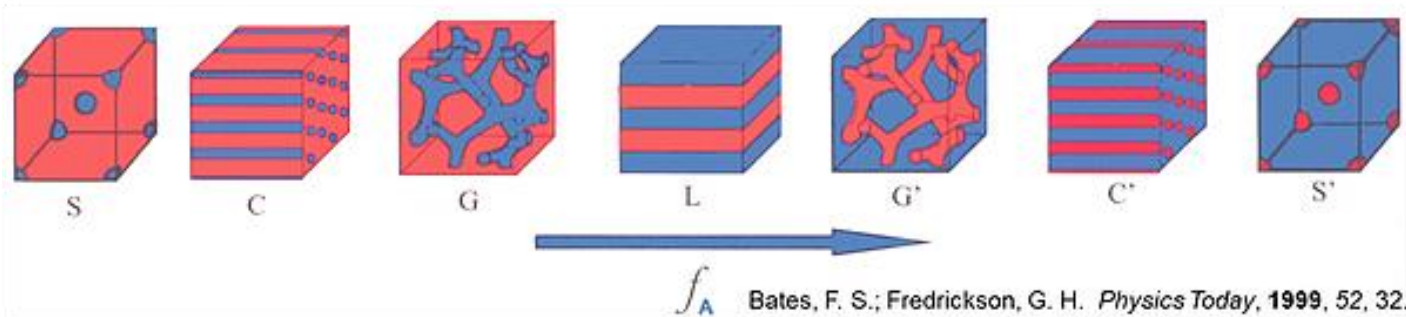
# Comparison of IPN and diblock copolymer

Classical microphase separation

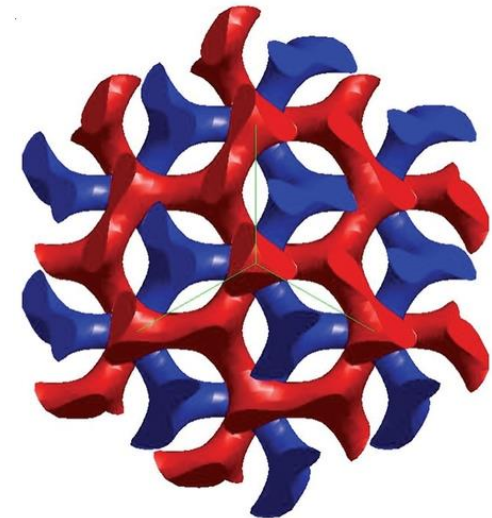
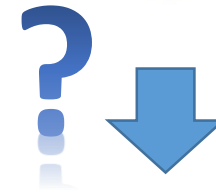
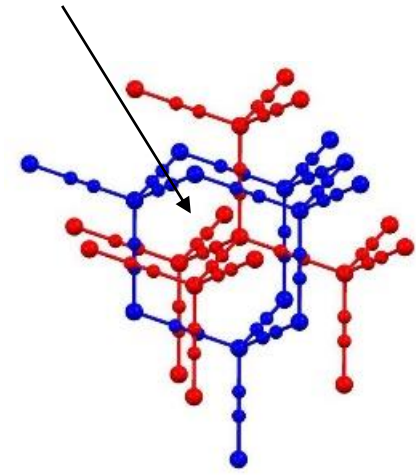


## Key Parameters

- $f$  volume fraction of each block (composition)
- $N$  degree of polymerization (size)
- $\chi$  interaction parameter (compatibility)



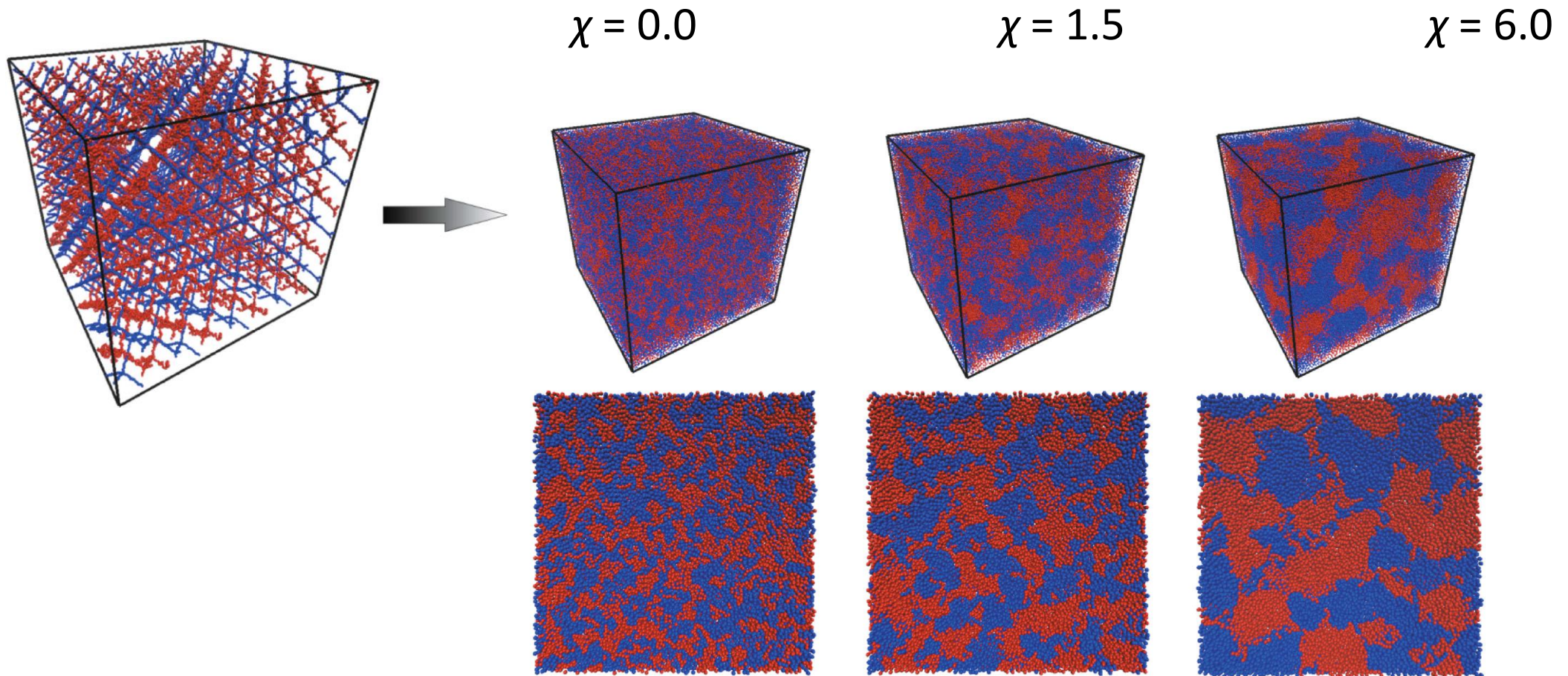
Topologically entangled



Is it possible to obtain microphase separation for topologic, not covalent entanglements?

# IPN rubber

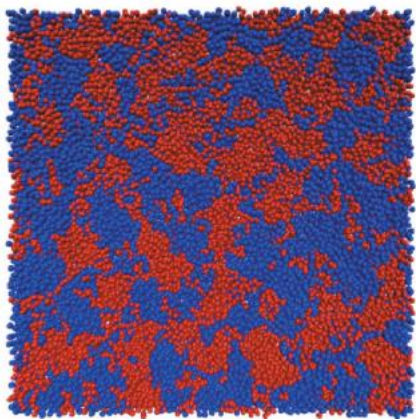
Influence of subnetworks compatibility (Flory-Huggins  $\chi$  parameter)



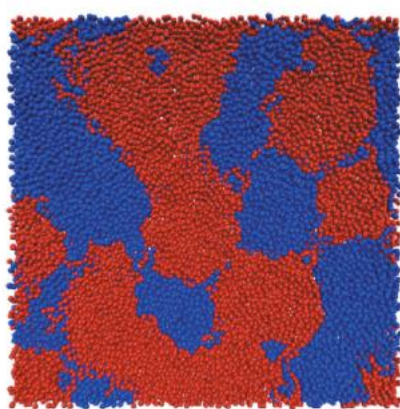
In contrast with diblock copolymers, no microphase separation with long range order is possible!

# IPN rubber: influence of mesh size

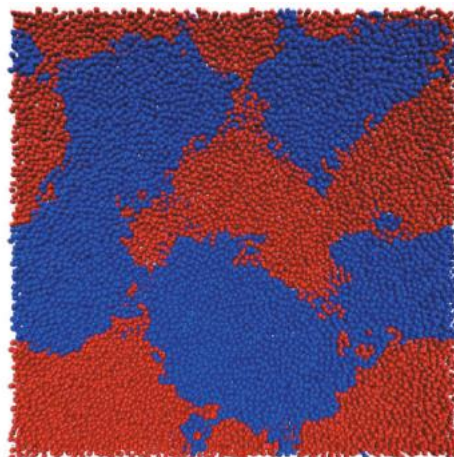
$l_1=l_2 = 10$



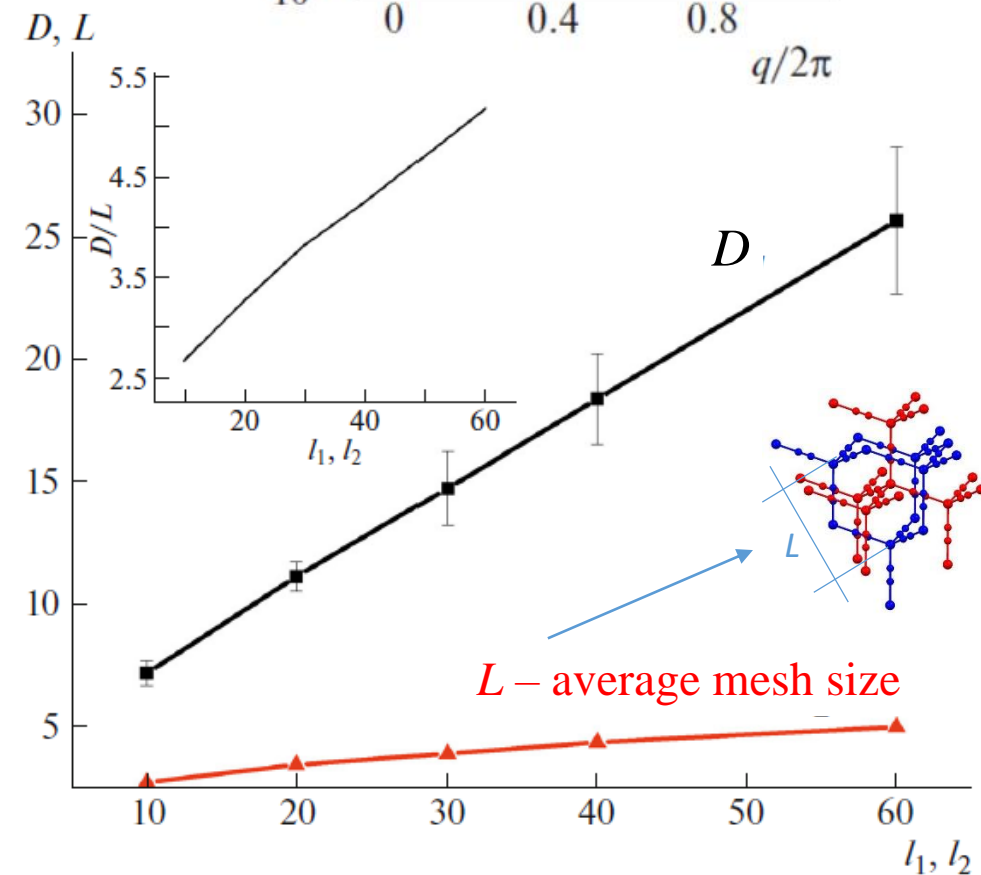
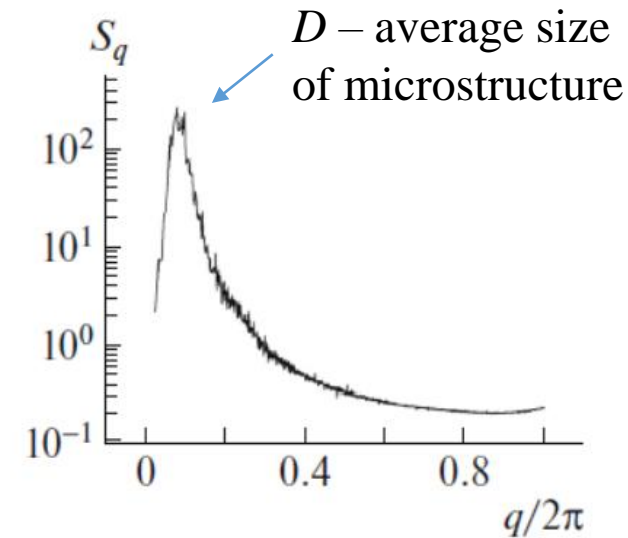
$l_1=l_2 = 30$



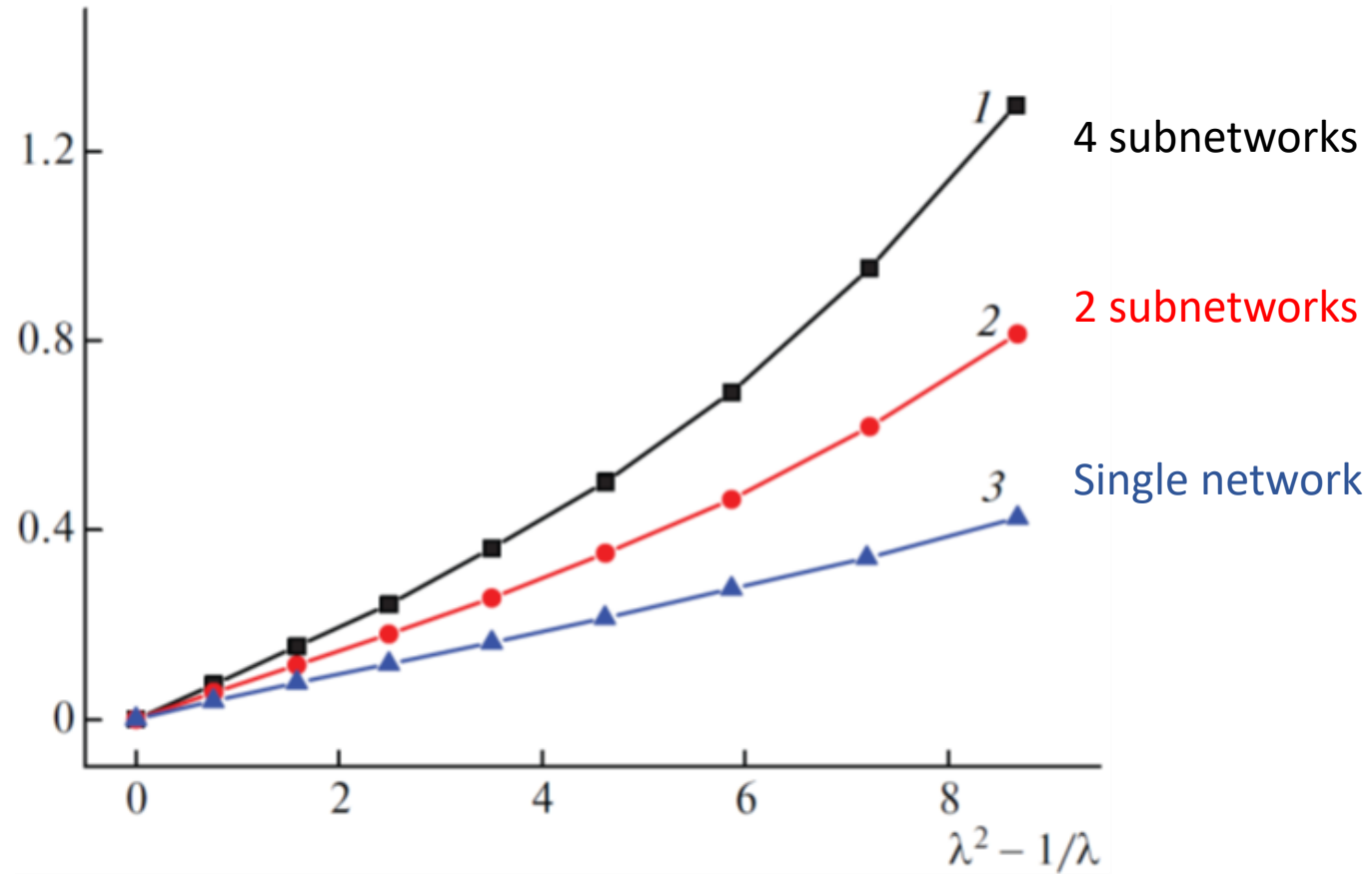
$l_1=l_2 = 60$



IPN topological entanglements are “sliding” and do not correspond directly to mesh size, so no special size is preferable during fluctuations.



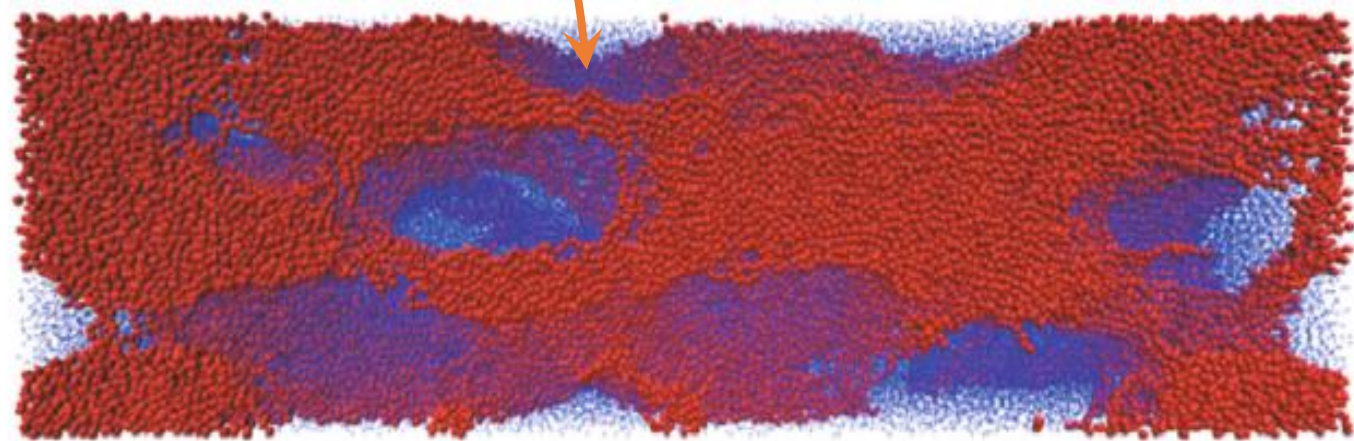
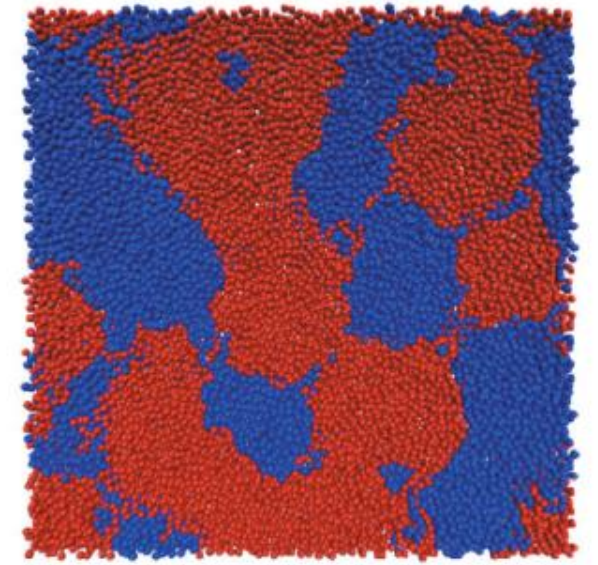
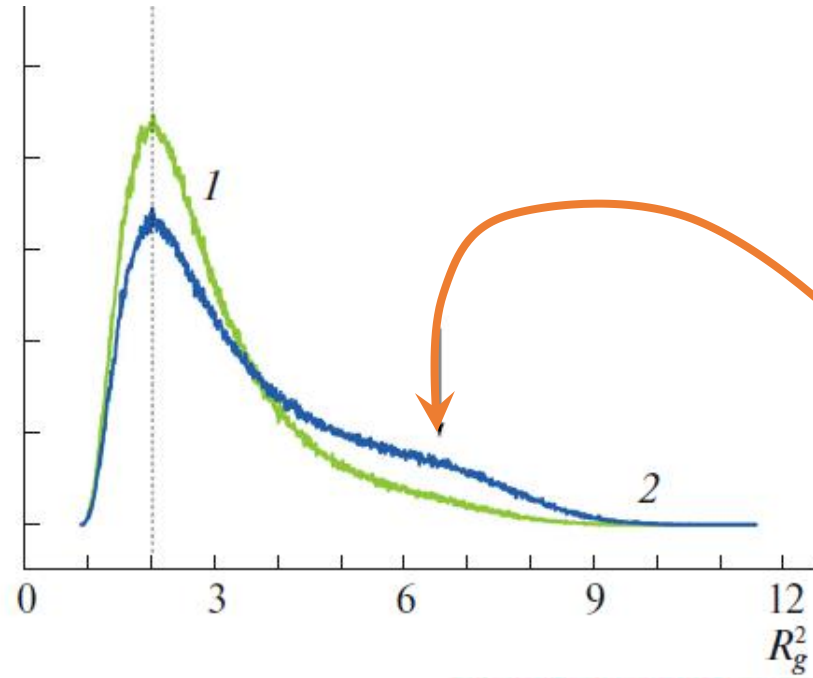
# Influence of subnetworks number on IPN rubber elasticity



The more subnetworks the more strong and nonlinear stress-deformation

This is the effect of smaller fraction of elastic-active subchains

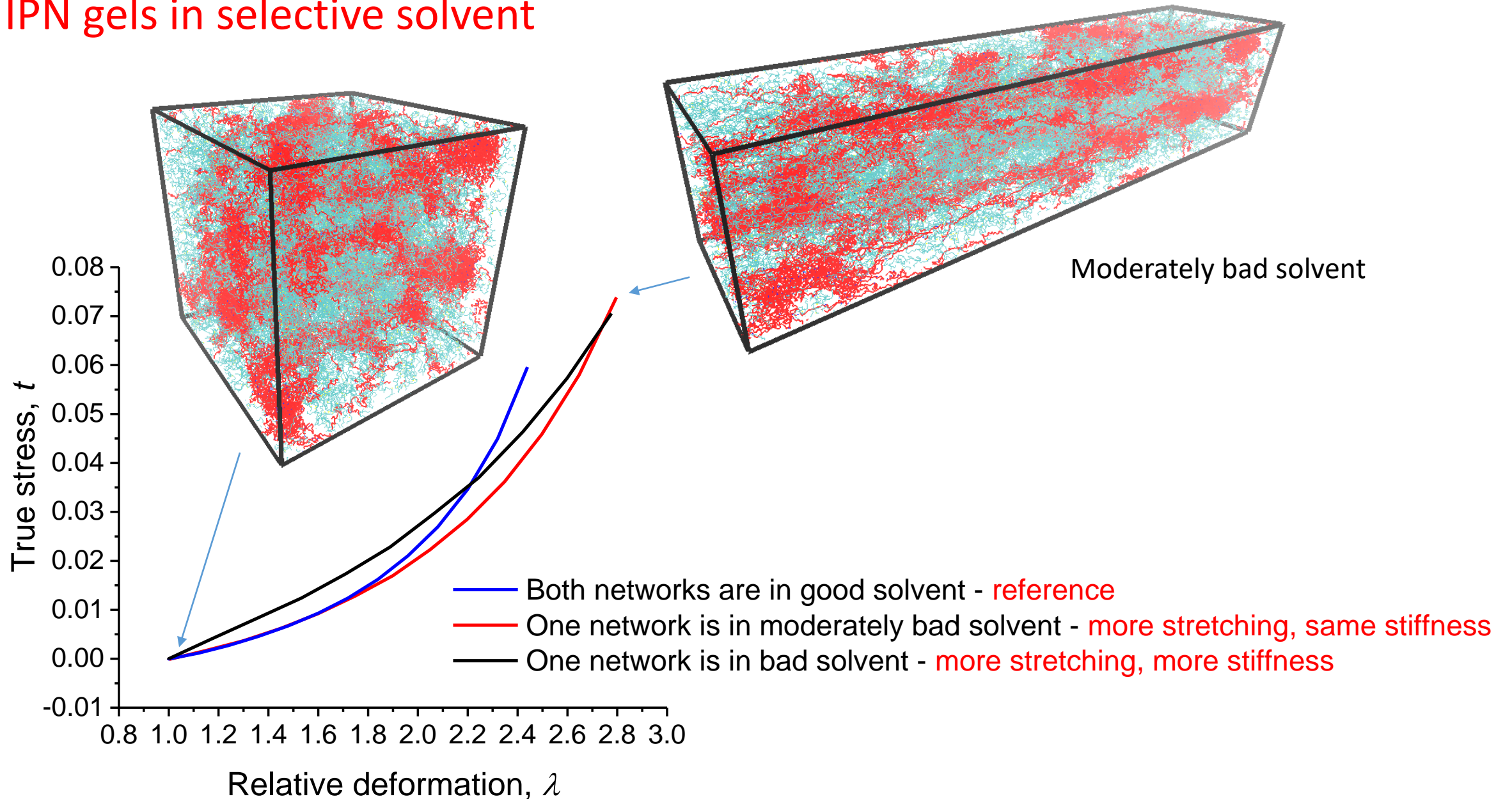
# Deformation of partly segregated IPN rubber



Partly segregated subnetworks have special fraction of very deformed subchains

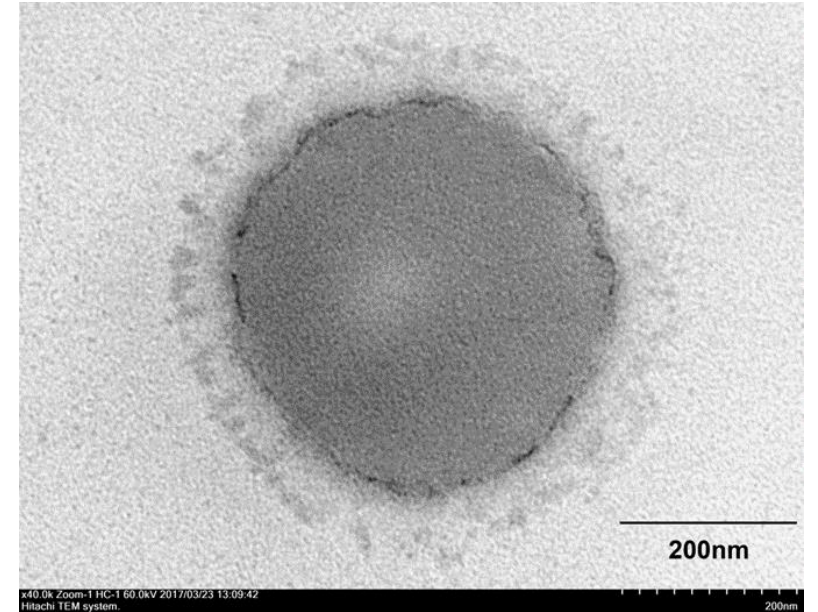
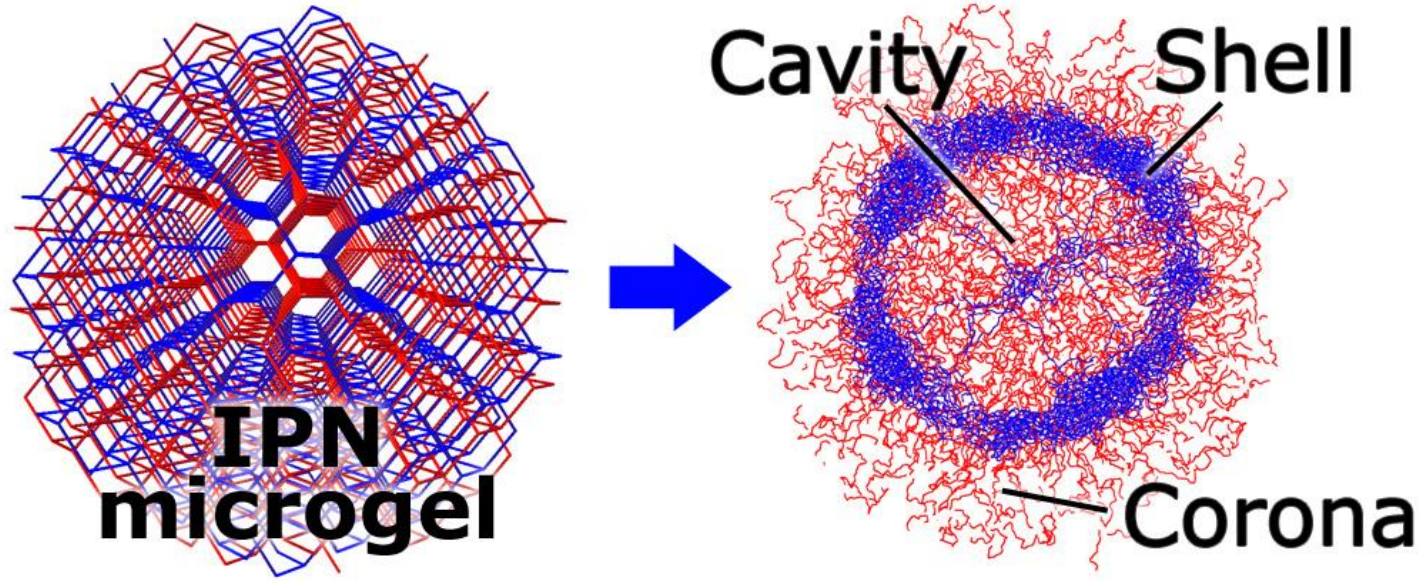


# IPN gels in selective solvent



Selective solvent in IPN gel can control its toughness and elasticity!

## IPN Microgel in selective solvent

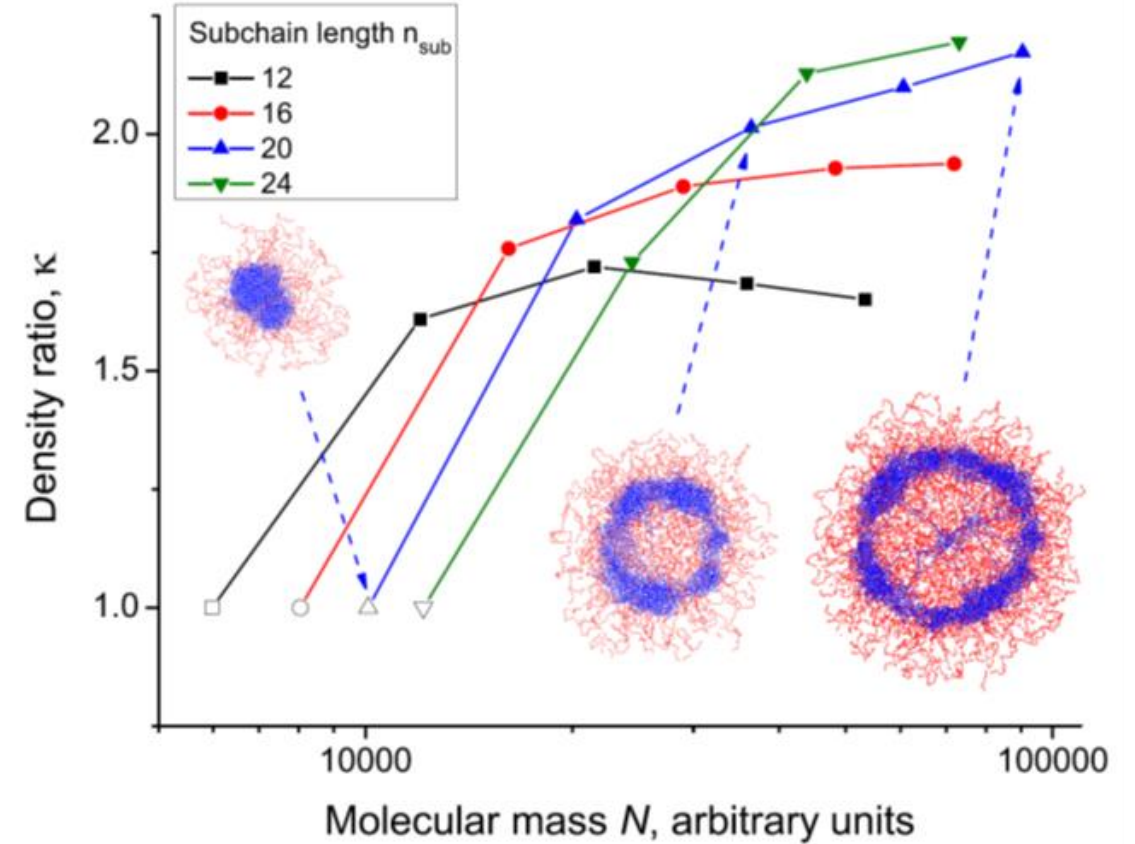
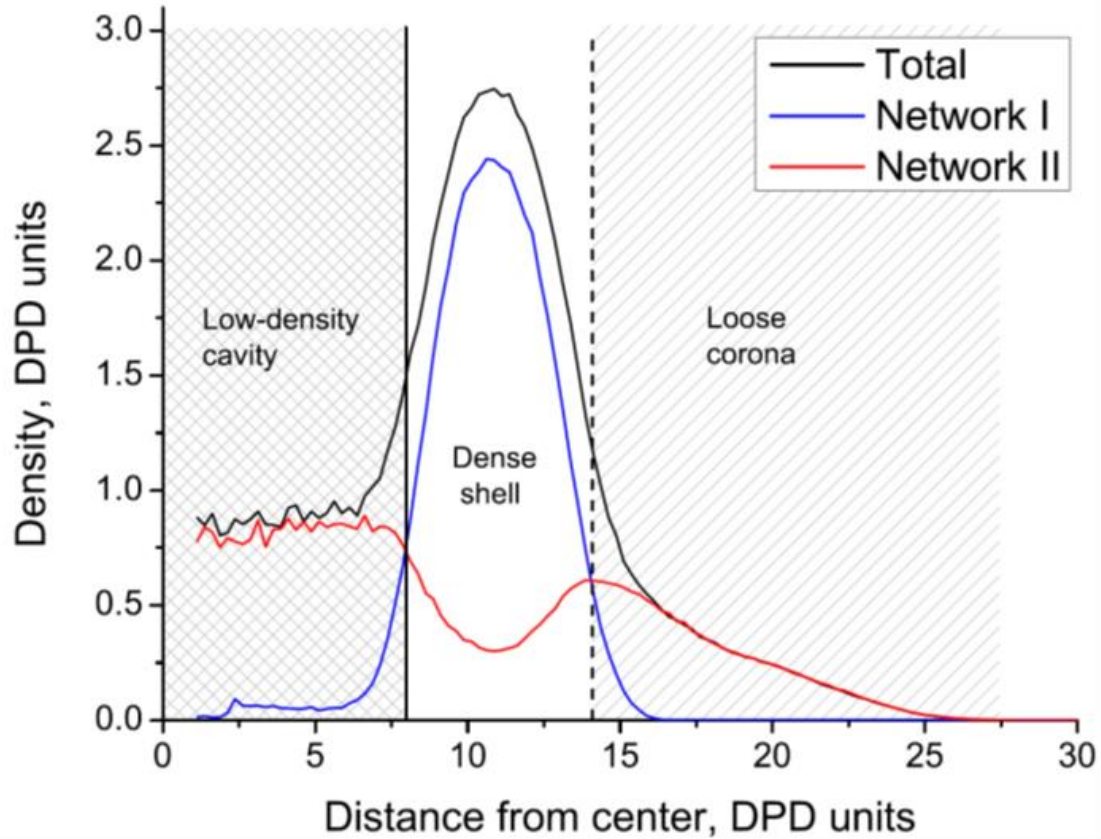
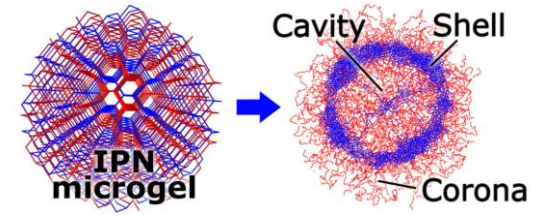


Experimental example: PNIPA + PAA = pH + Temperature sensitivity

Poster 4\_303 by Elena Kozhunova

Set of topological entanglements prevents the collapse of blue network into a single core

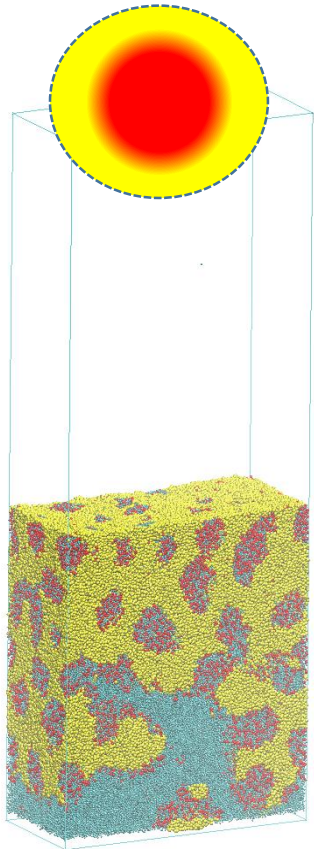
# IPN Microgel in a selective solvent



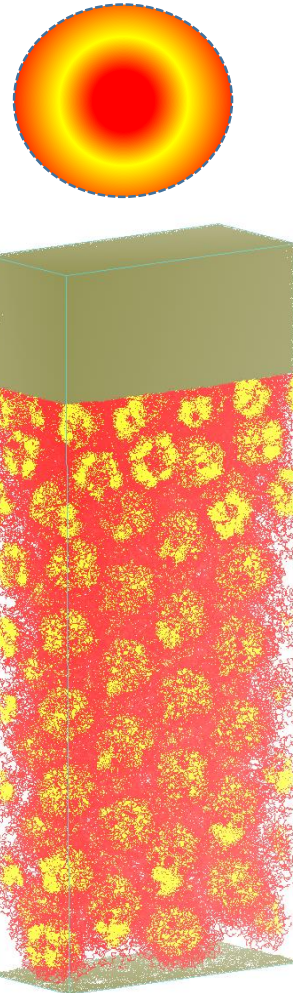
This is size-dependent effect, work only for large mesh size or small gel size

# IPN Microgel as small molecules container

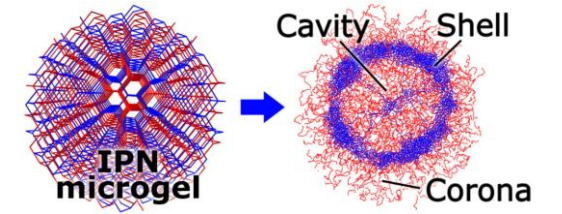
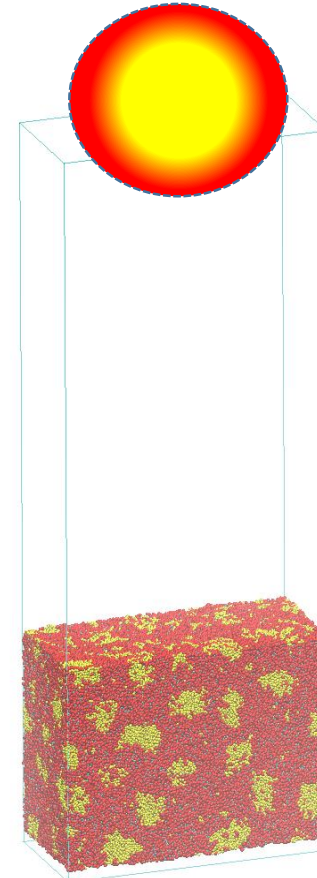
Hydrophilic core –  
hydrophobic shell  
Microgel



IPN Microgel



Hydrophobic core  
– hydrophilic shell  
Microgel



- No aggregation
- No guest molecules leakage

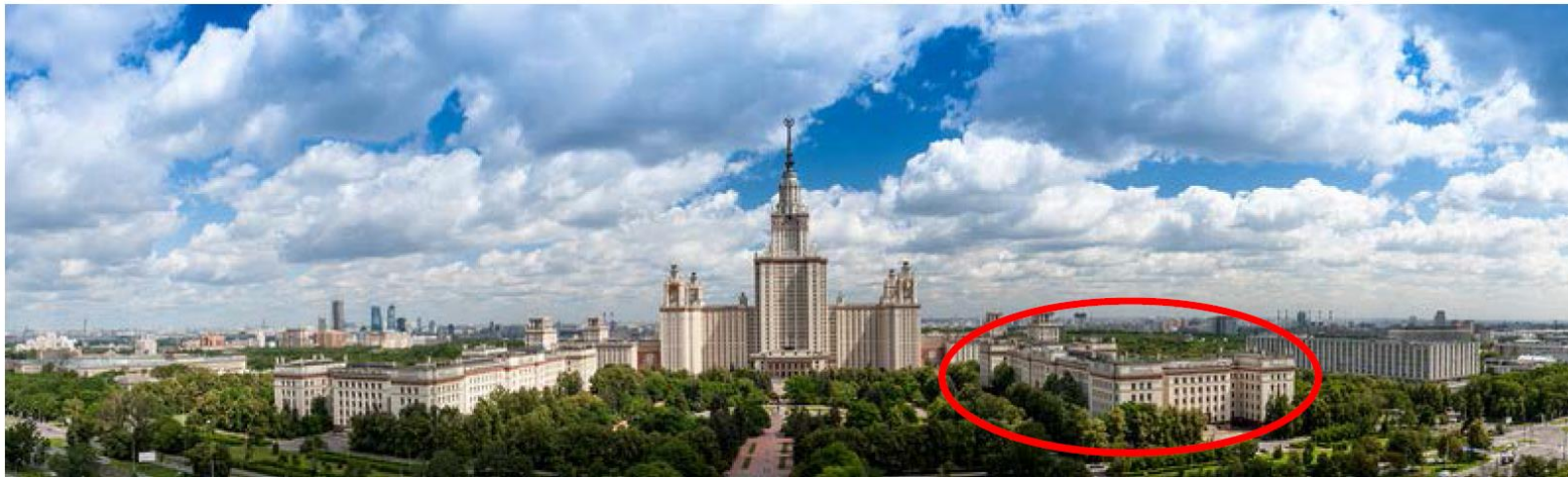
- hydrophilic
- hydrophobic
- solvent
- vapor

IPN microgel could be used as universal container for many different guest molecules

# Acknowledgements: Alexey Gavrilov, Vladimir Rudyak, Pavel Kos



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