# POLYMER NETWORKS: MODELING AND EMERGING APPLICATIONS

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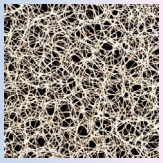
## BACKGROUND

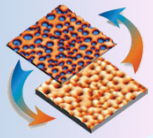
**Polymer networks** are natural, synthetic, or hybrid natural-synthetic materials in which constituting polymer chains are all connected to each other either directly or via other connecting chains.

Actin network



Schmoller *et al.*, Nature Communications, 2010

- **Properties of polymer networks**
  - Highly permeable (porosity $\sim 0.75 - 0.98$)
  - Extremely flexible (modulus $\sim 1 - 10^3$ kPa)
  - Mechanically sturdy (support external loads)
  - Sensitive to external stimuli (light, pH, temperature, etc)
- **Applications of polymer networks**
  - Active and responsive systems
  - Drug delivery
  - Lubrication

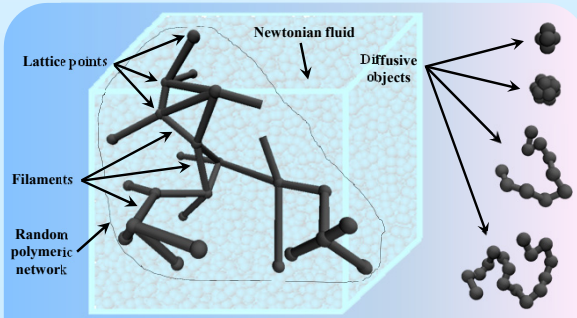


Tokarev and Minko Adv. Mater., 2010

## OBJECTIVES

- **Develop a model for liquid-swellable polymer networks**
- **Apply the model to examine the permeability and diffusivity of initially isotropic networks with different porosity and internal structure under normal and shear loadings**
- **Employ the model to study the effect of swelling and deswelling volume transitions on the release of encapsulated nanopaticles from hollow microgel capsules**
- **Use the model to examine approaches for regulating friction between gel-coated surfaces**

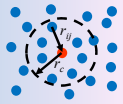
## SIMULATION SETUP



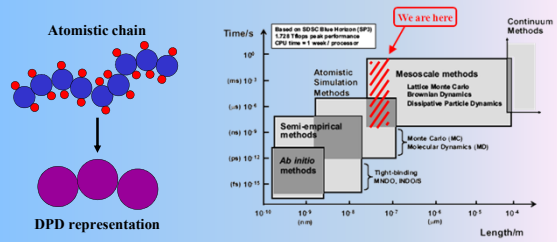

- **Use DPD to simulate transport through random lattice of interconnecting filaments as model for polymer networks**

## DISSIPATIVE PARTICLE DYNAMICS

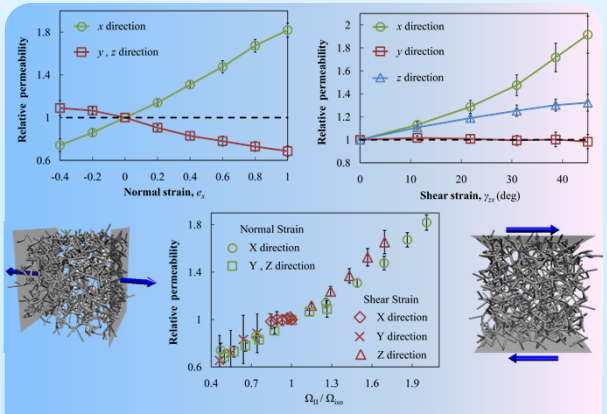
- **Newtonian time evolution of many-body system (similar to MD)**
  - Repulsive forces (accounts for compressibility)
  - Dissipative force (mimics viscosity)
  - Stochastic force (represent thermal fluctuations)



- **Pair-wise and central forces to preserve hydrodynamics**
- **Departure from MD:**
  - Soft conservative interaction potential ("fluid elements")
    - Allow simulations with larger time/length scales



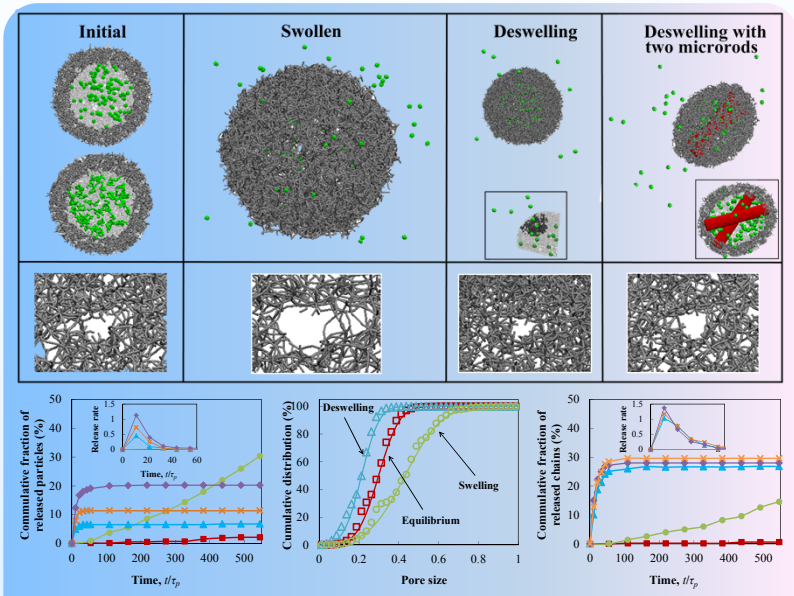

## RESULTS




- **Stretching enhances permeability in direction of deformation**
- **All data collapses into single master curve in principal directions**

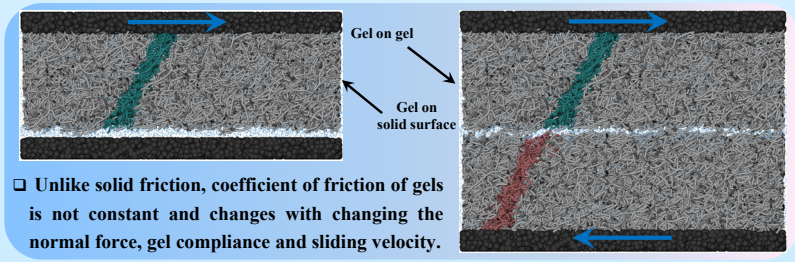
Permeability and diffusion through mechanically deformed random polymer networks
**Masoud** and Alexeev, ***Macromolecules*** 43, 10117 (2010)

## RESULTS CON'T




- **Release from swollen capsules is relatively slow and is controlled by diffusion**
- **Deswelling induced release is driven by fluid flow from inside capsule through membrane and is limited by network mesh size at long times**
- **Polymer chains are released faster than rigid particles during capsule deswelling whereas particles diffuse out of swelling capsule faster than polymer chains**

Controlled release of nanoparticles and polymer chains from responsive microgel capsules
**Masoud** and Alexeev, ***ACS Nano***, Under review (2011)




- **Unlike solid friction, coefficient of friction of gels is not constant and changes with changing the normal force, gel compliance and sliding velocity.**

Friction between gel-coated sliding surfaces
**Masoud** and Alexeev, In preparation