

Active Control of Polymer Structure

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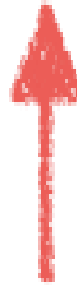
Indian Institute of Science Education and Research Bhopal

SWPNIOE 2026

What is active matter?



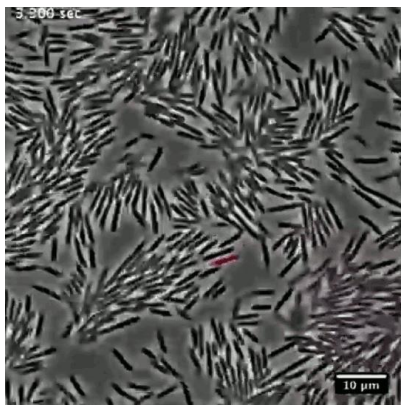
Meter scale
Inertial forces dominate



Micro meter scale
Viscous forces dominate

Active matter:
Particles are *engines*

Driven matter:
Particles are *passengers*



Supplementary video S2:
Active particle driven
clustering of passive particles

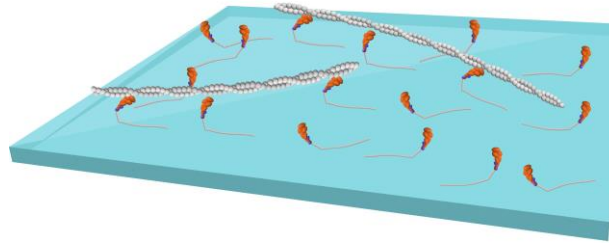


Bacteria colony

Active polymers and filaments



Bacterium

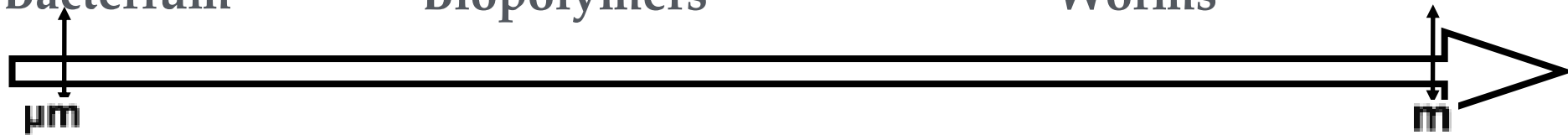


Biopolymers



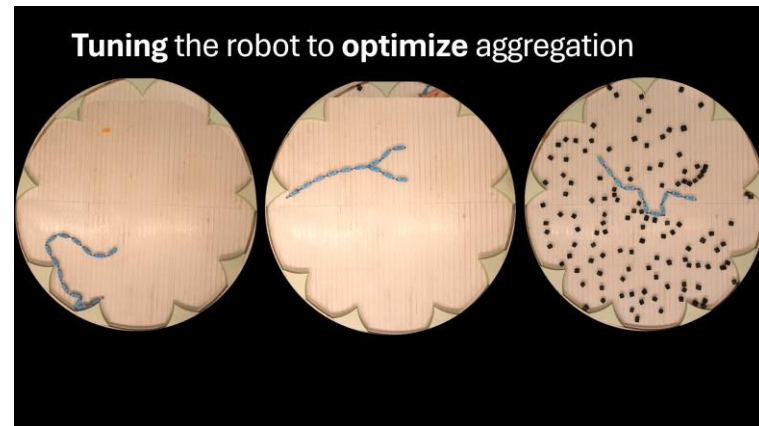
Worms

Biological
systems



Colloidal caterpillar

Soft Matter, 2014, 10, 8813–8820



Tuning the robot to **optimize** aggregation

Robotic filament

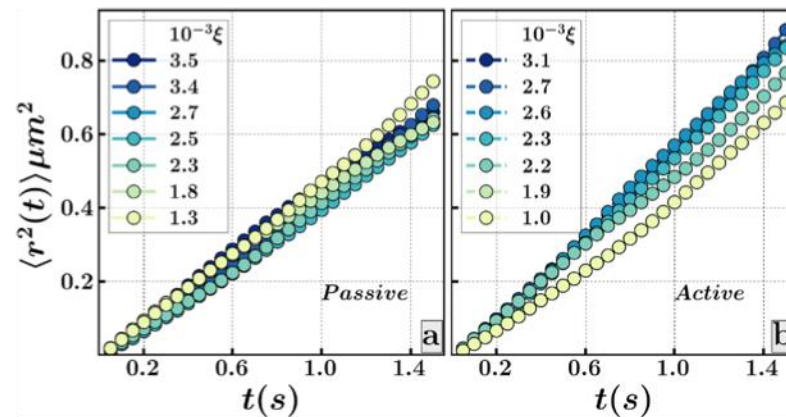
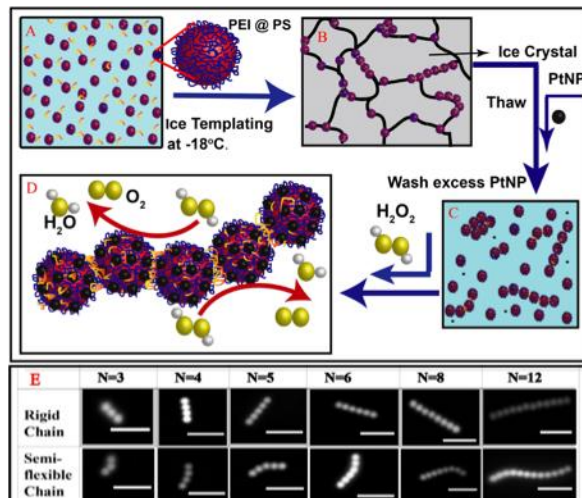
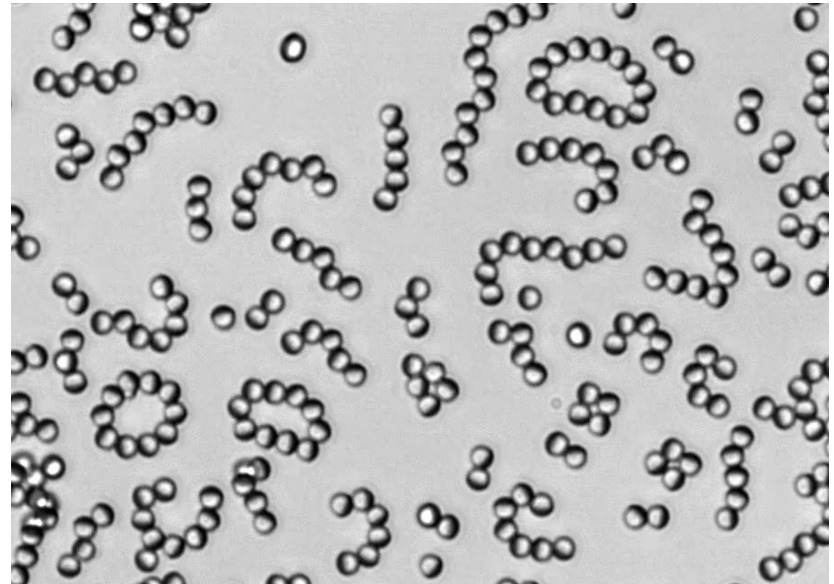
Phys. Rev. X, 2026, 16, 011003

Bio-
inspired
systems

- Elongated and flexible/semi-flexible
- Self-propelled

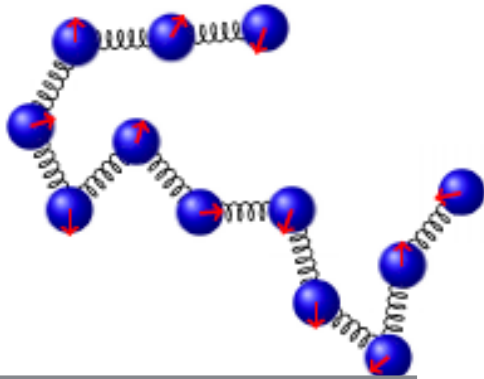
Phoretically active filaments

New J. Phys. 20, 015002 (2018)



Various active force profile along the filament

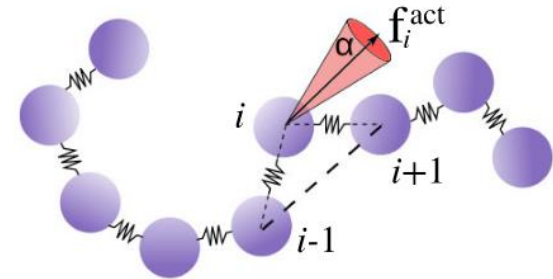
Active Brownian polymer (ABPO)



J. Chem. Phys. 141, 044903 (2014)

PRE, 101, 030501 (2020)

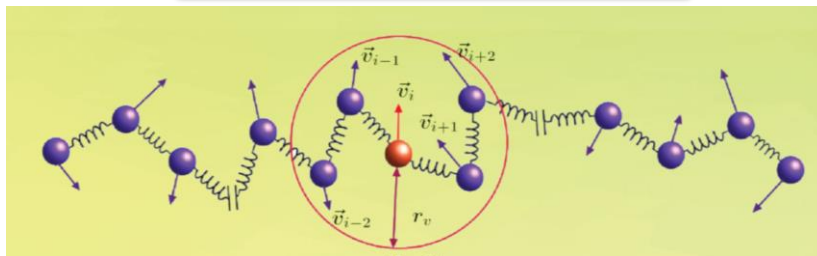
Polar active filaments



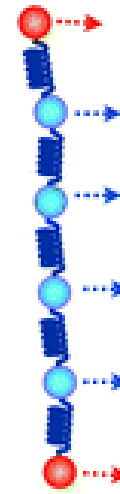
PRL 121, 217802 (2018)

Transversally propelling polymer

Alignment activity

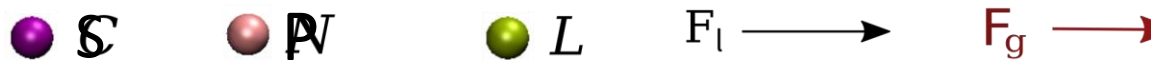
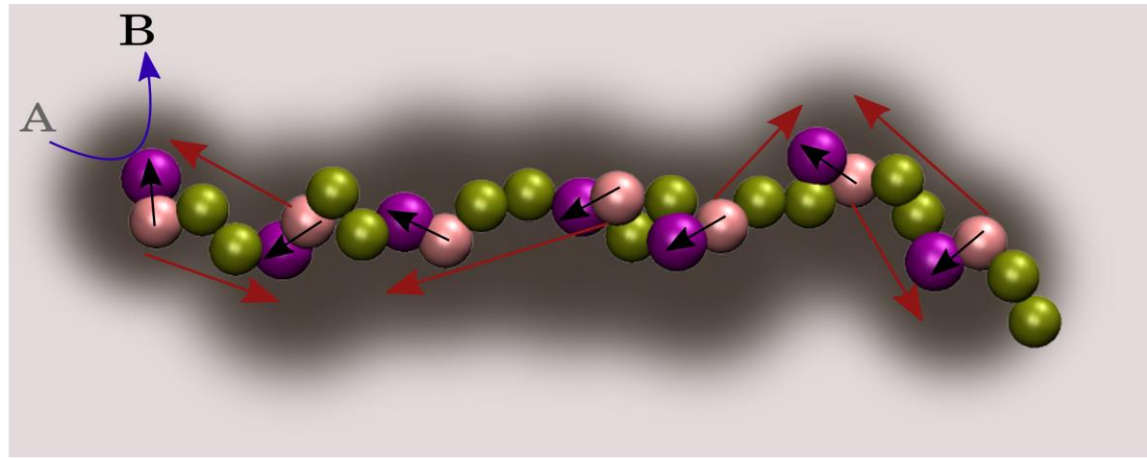


Soft Matter, 18, 1978 (2022)



Soft Matter, 18, 2928 (2022)

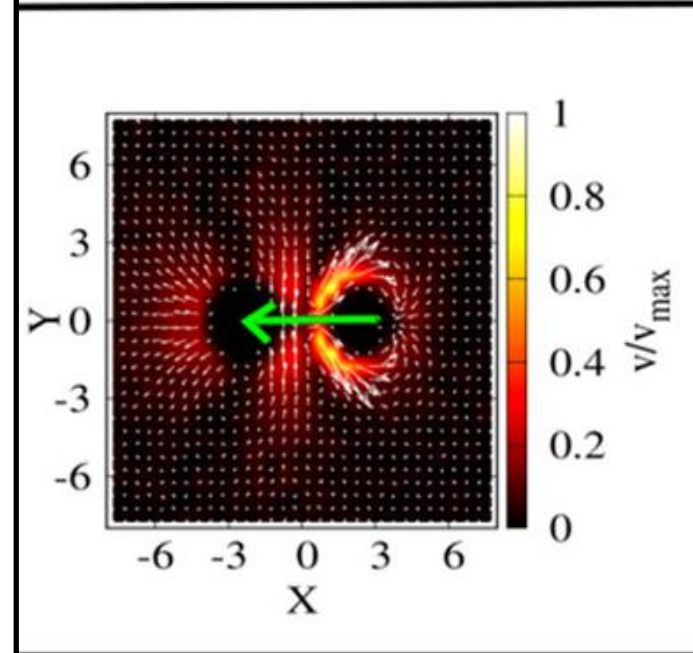
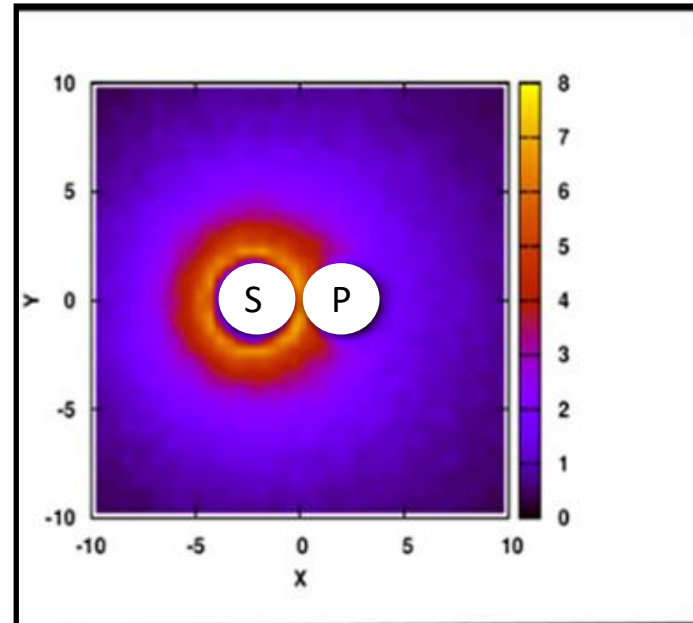
Phoretic active flexible polymer



S : Chemically Active (Source)

P : Chemically passive (Phoretic)

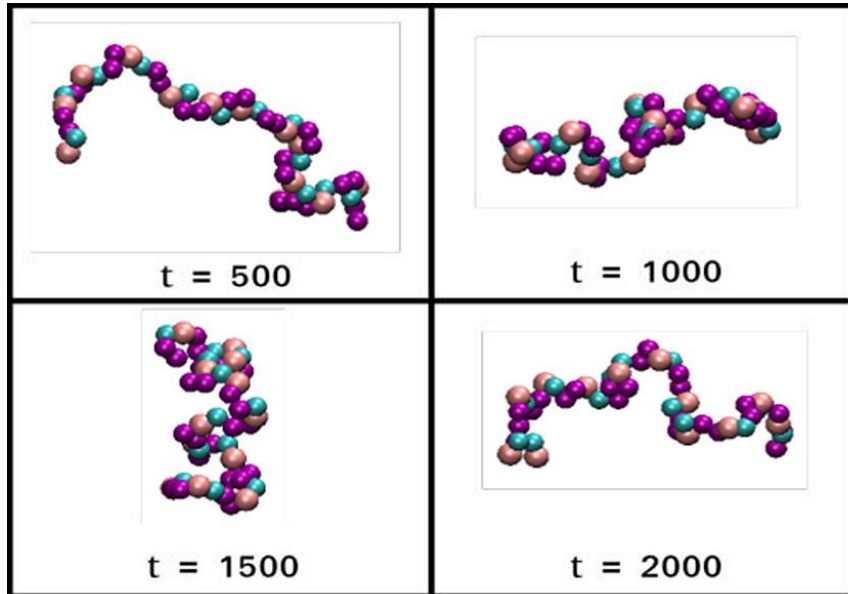
L : Linker (inactive)



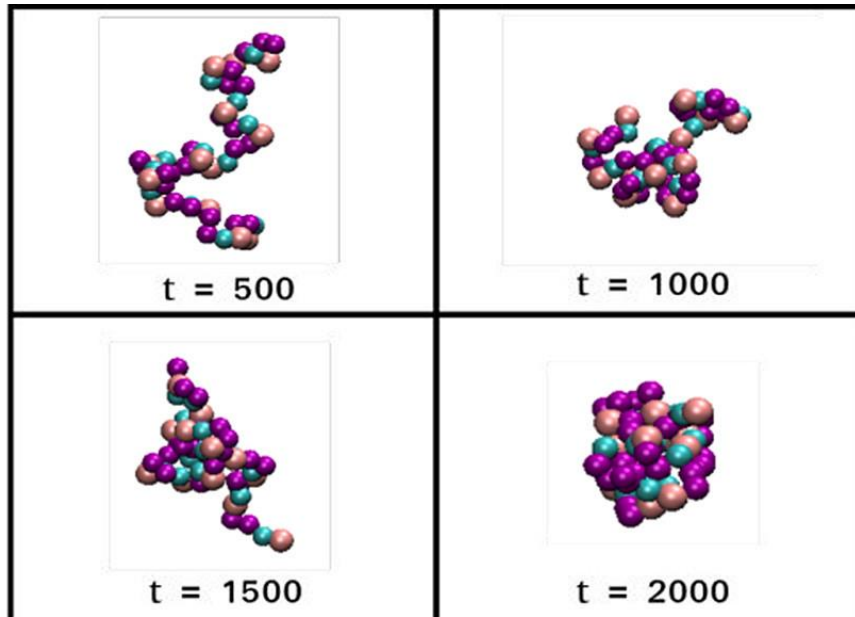
Active force due to diffusiophoresis

$$Pe = \frac{\epsilon_a}{\epsilon_b} \frac{\epsilon}{k_B T}$$

Influence of activity



Passive Polymer

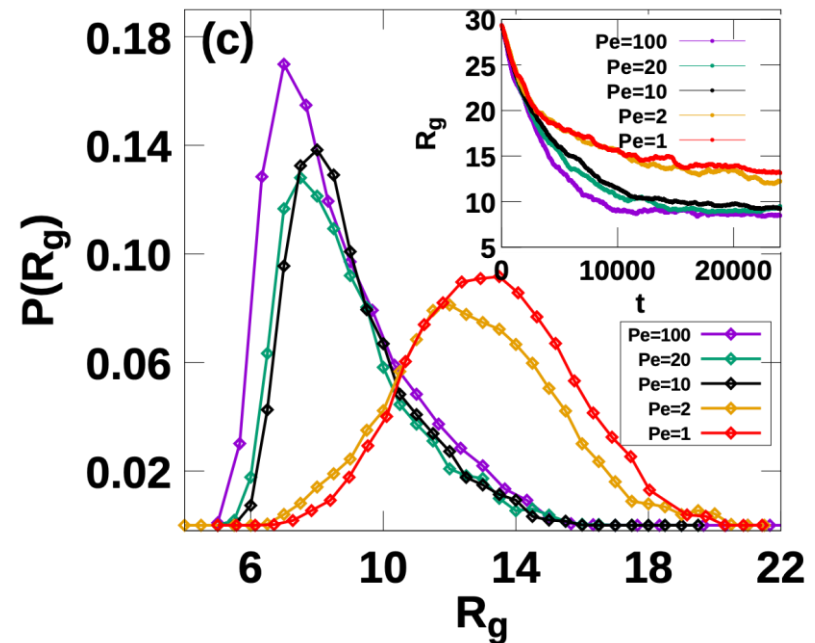
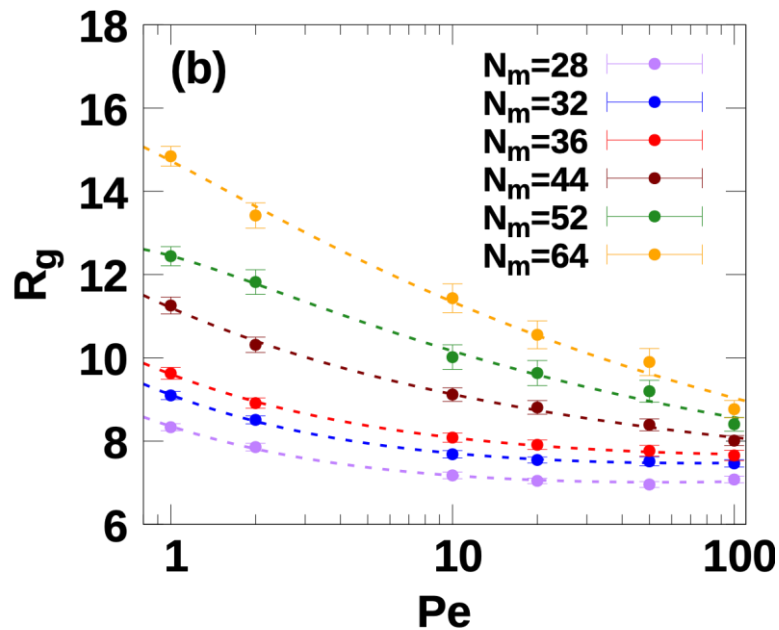


Active Polymer

The coil-to-globule transition is observed in active polymer

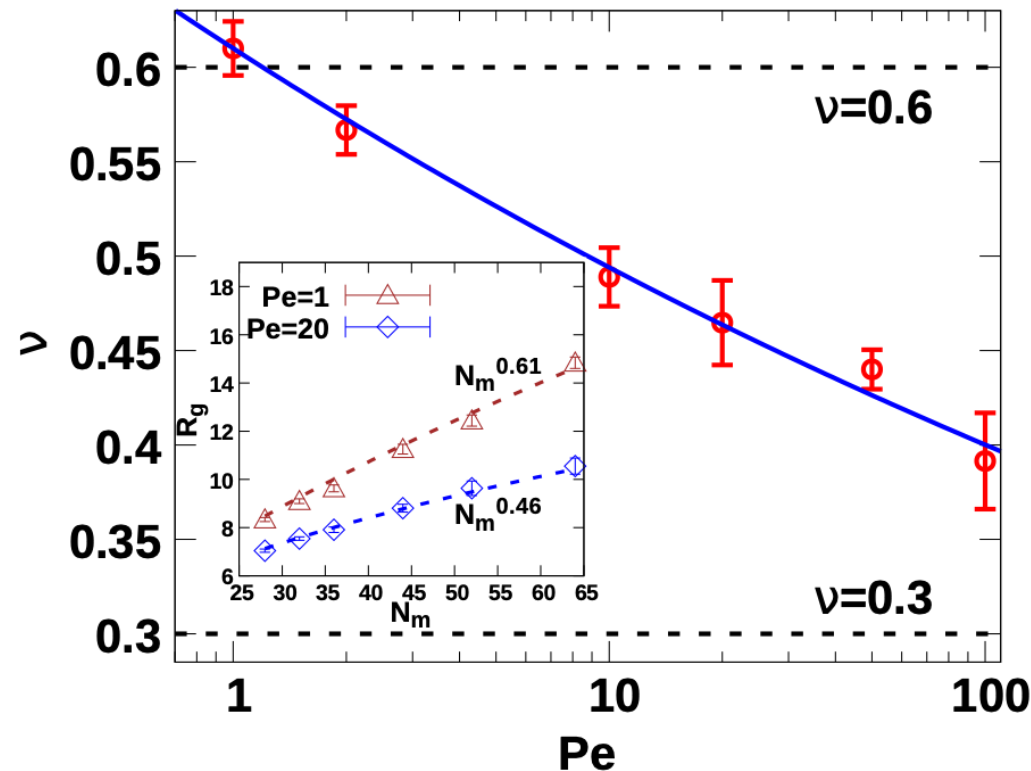
Influence of activity

$$R_g = \sqrt{\frac{1}{N_m} \left\langle \sum_{i=1}^{N_m} (\mathbf{r}_i - \mathbf{R}_{cm})^2 \right\rangle}$$



Emergence of compact globule state due to chemical activity

Flory exponent



$$\nu(Pe) = 0.61Pe^{-0.091}$$

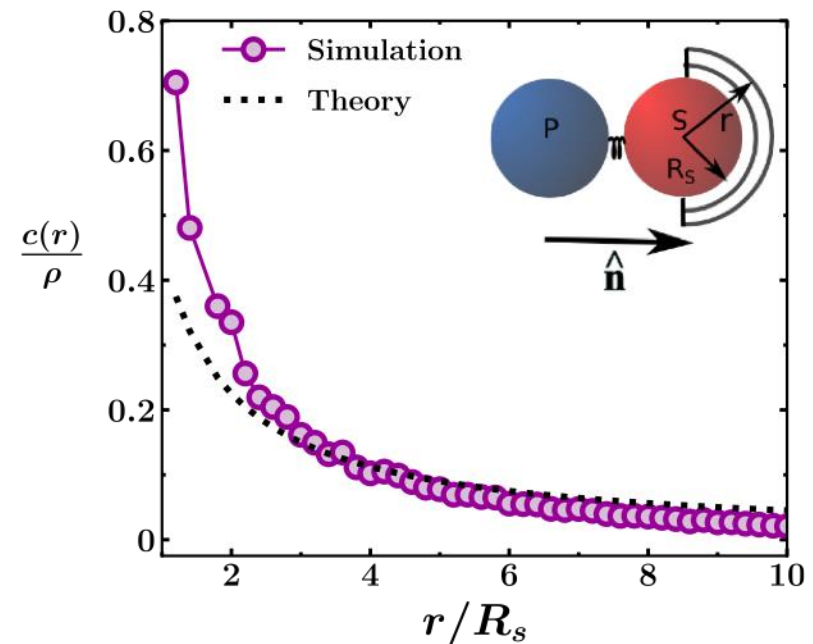
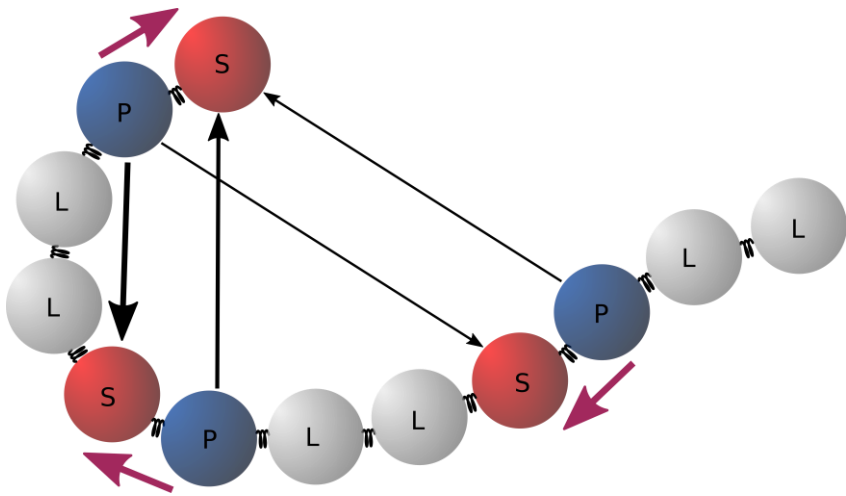
$$R_g = \sigma \frac{a_{R_g} + b_{R_g} \ln(Pe)}{(Pe + 1)^{c_{R_g}}} N_m^{\nu(Pe)}$$

Tangential force also shows the similar behaviour

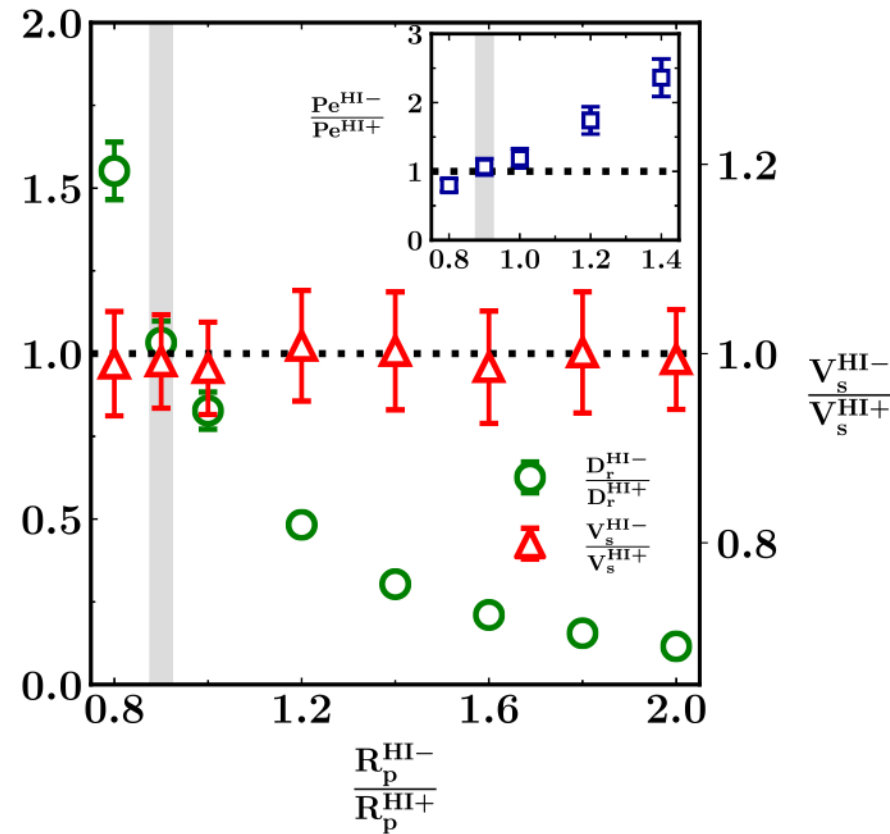
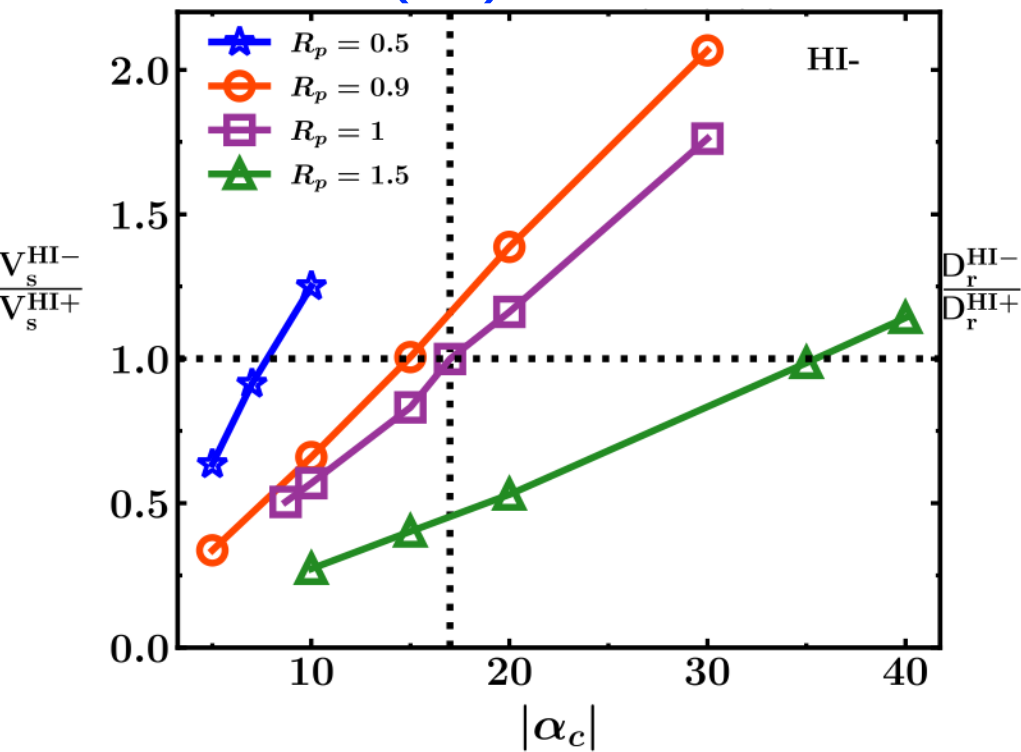
Coil-to-globule transition in a limited range of sizes

Diffusiophoretic Brownian Dynamics: Hydrodynamic Interaction (HI) Effect

- What about long polymers and larger activities?
- Can we design an effective way of including the phoresis without explicit solvent?
- Quantify the effect of HI



Diffusiophoretic Brownian Dynamics: Hydrodynamic Interaction (HI) Effect

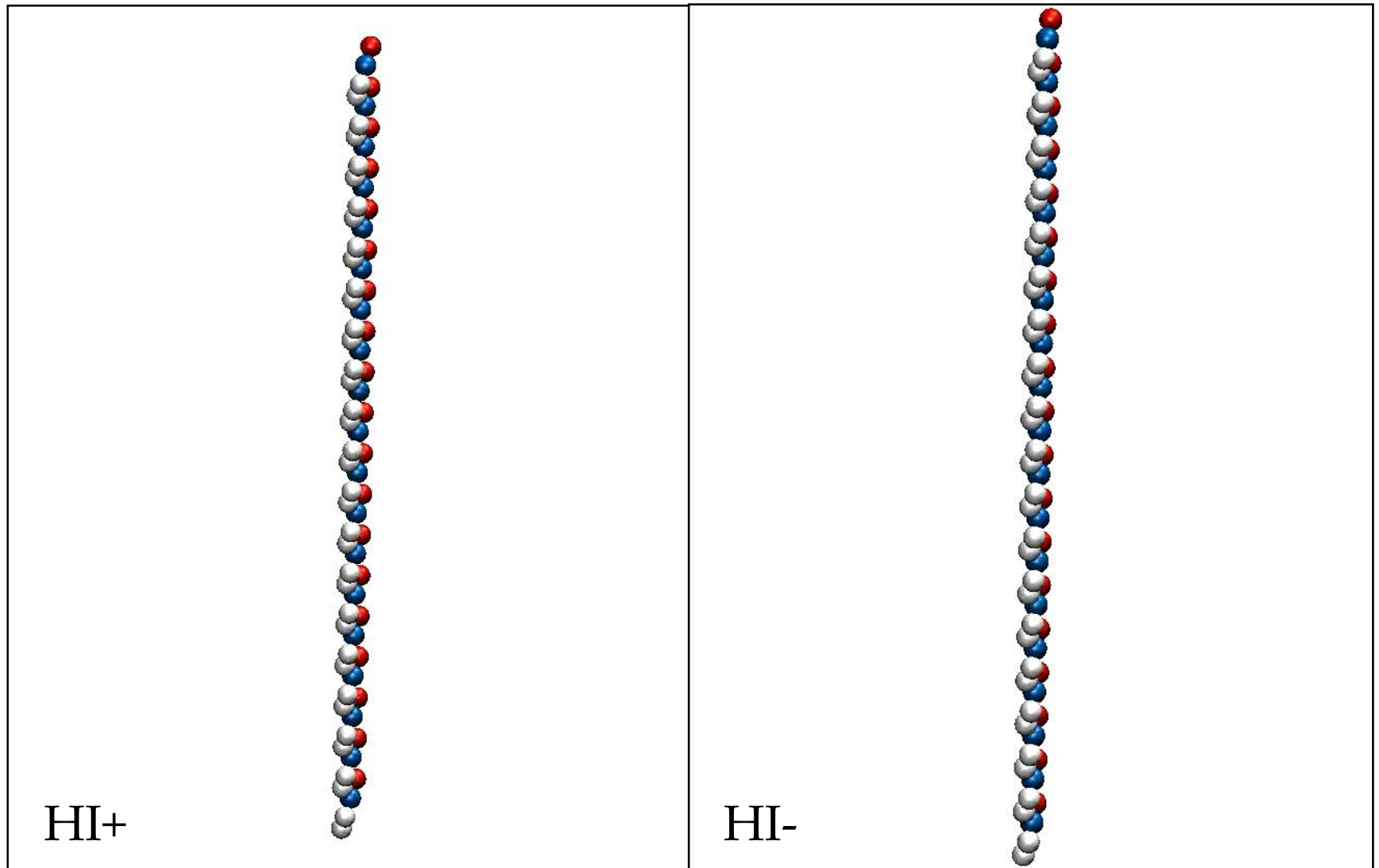


$$\mathbf{F}_{c,i}(\mathbf{r}_i) = -\alpha_c \frac{k_B T}{\rho} \nabla c(\mathbf{r}_i)$$

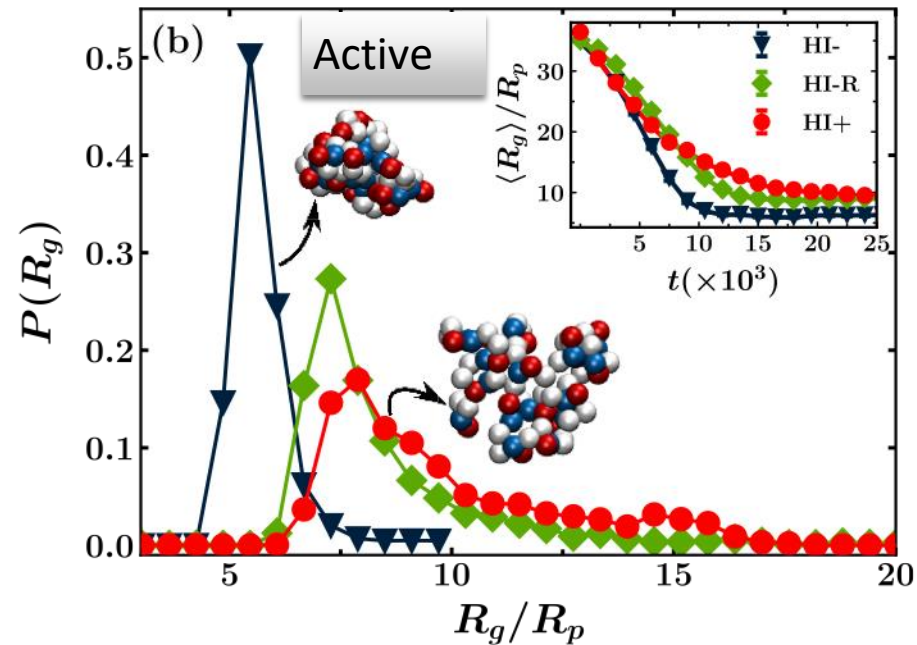
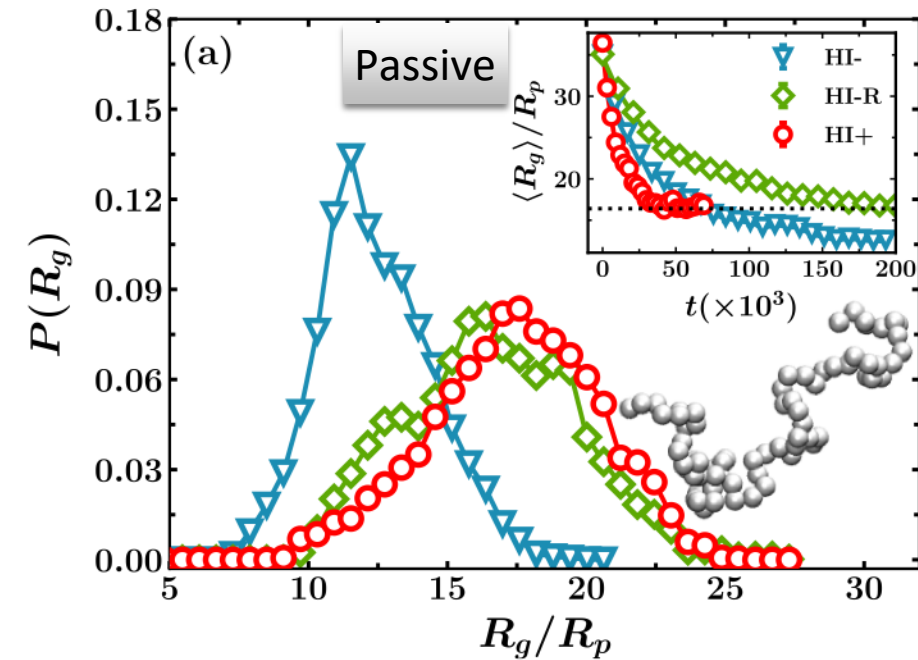
$$\nabla c(\mathbf{r}_i) = \sum_j \frac{\Delta c}{(r_{ij} + R_p)(r_{ij} - R_p)} R_s \hat{\mathbf{r}}_{ij}$$

$$Pe = \frac{V_s}{D_r R_p}$$

Active Polymer: HI^+ vs HI^-

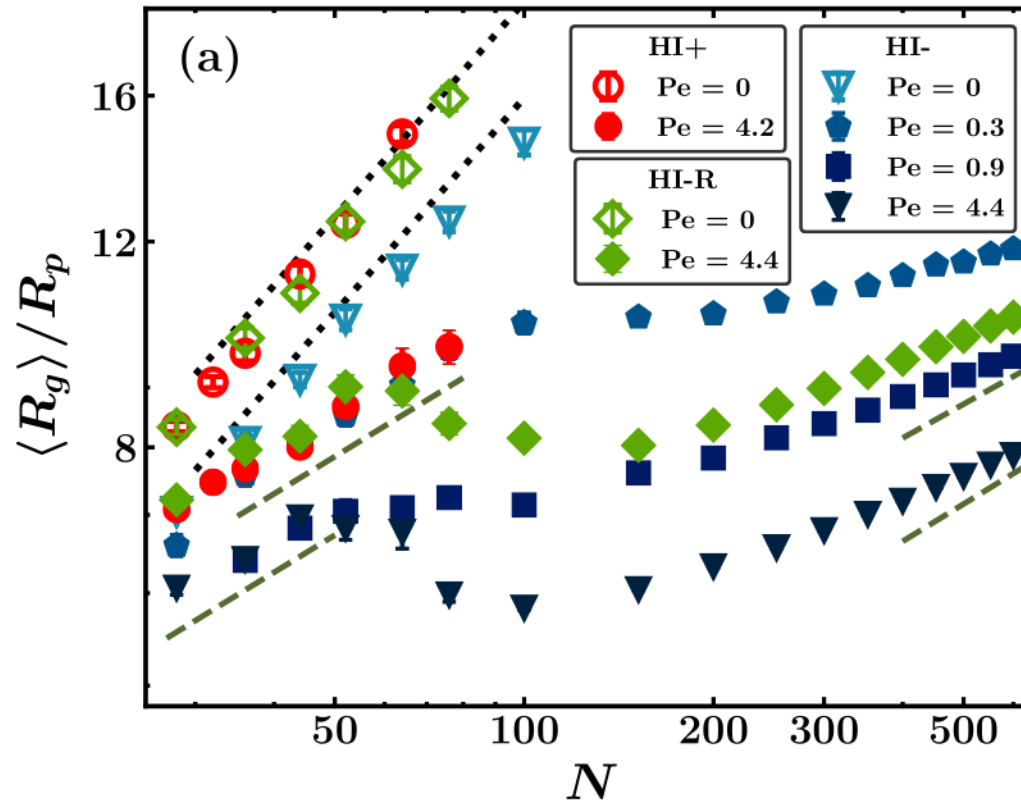


Effect of HI



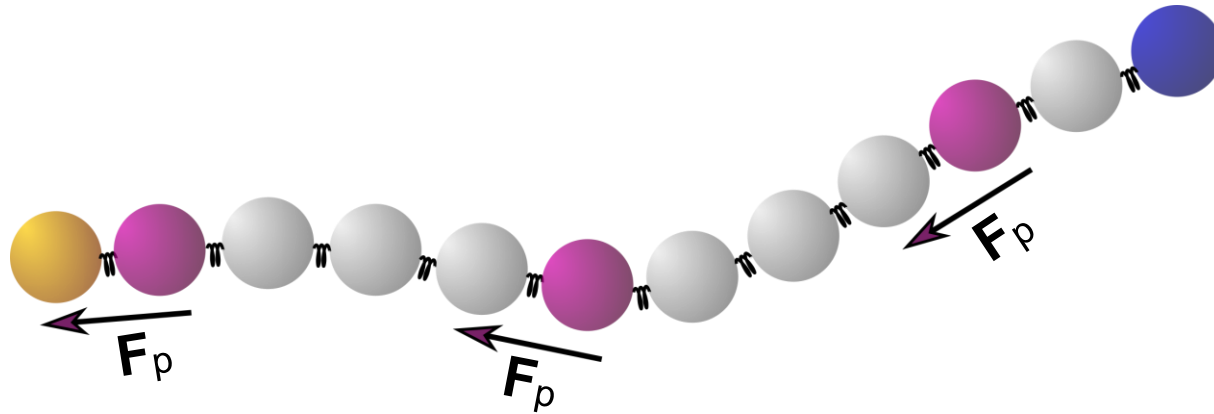
The larger R_g for HI+ can be due to an effective repulsion given by a solvation layer

Active Polymer: Dependence on Polymer Length

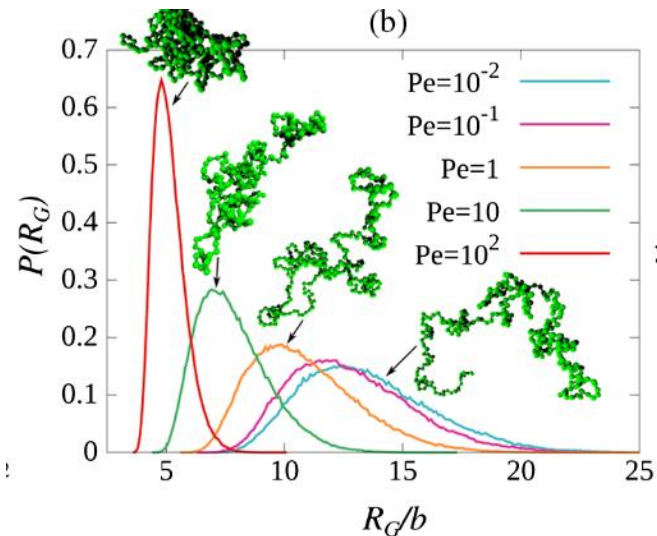


Nonmonotonic behavior is activity dependent and becomes stronger with

Polar active polymers



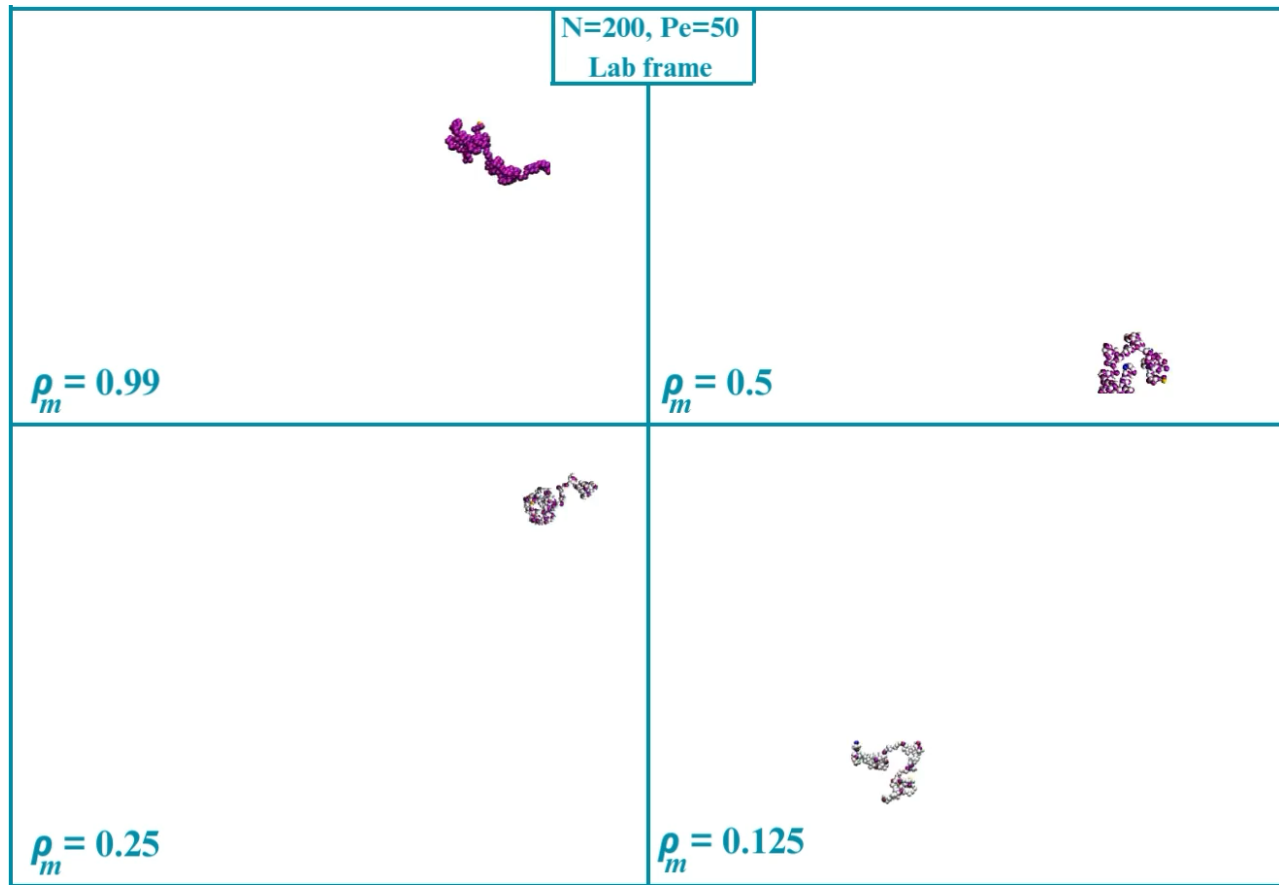
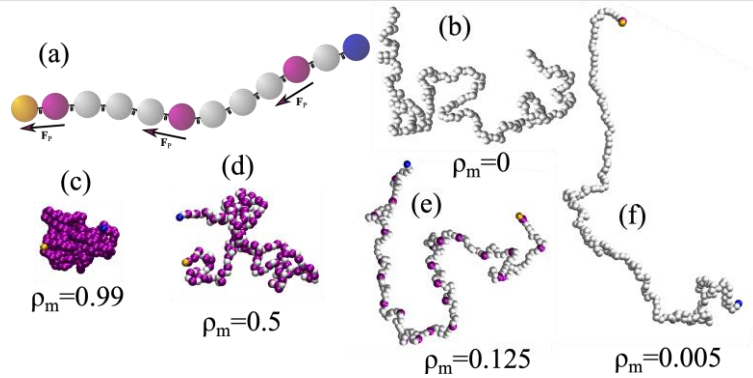
When all constituent monomers are active



PRL 121, 217802 (2018)

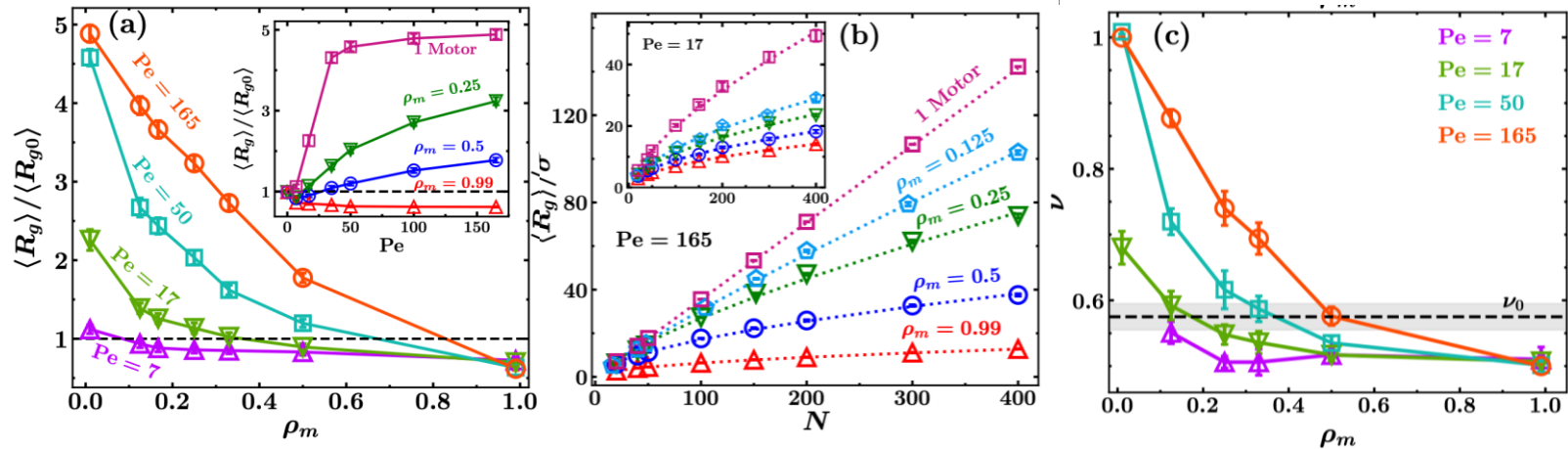
- But.... in biopolymers, synthetic polymers, activity is localised
- ~20% of the total genes are transcriptionally active at a given time

Polar active polymers: role of the motor density



Less density leads to stretching

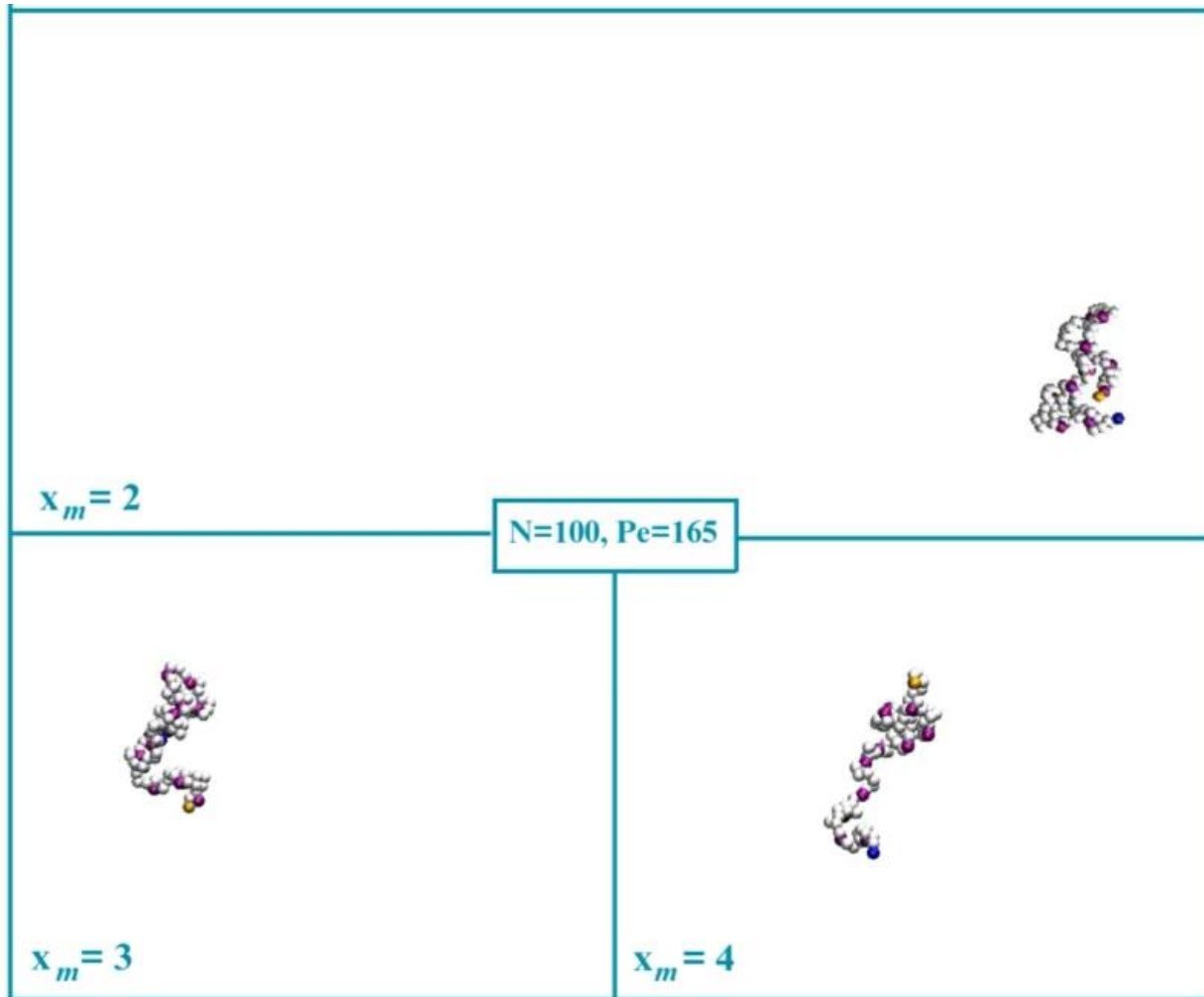
Polar active polymers: role of the motor density



- Small activity compactify the polymers, opposite to larger activities for which the polymer stretches
- $R_g \sim N^\nu$, Scaling exponent = 0.6 for passive polymer
- $\nu < \nu_0$ compact states
- $\nu > \nu_0$ stretched state

Polar active polymers: role of the motor position

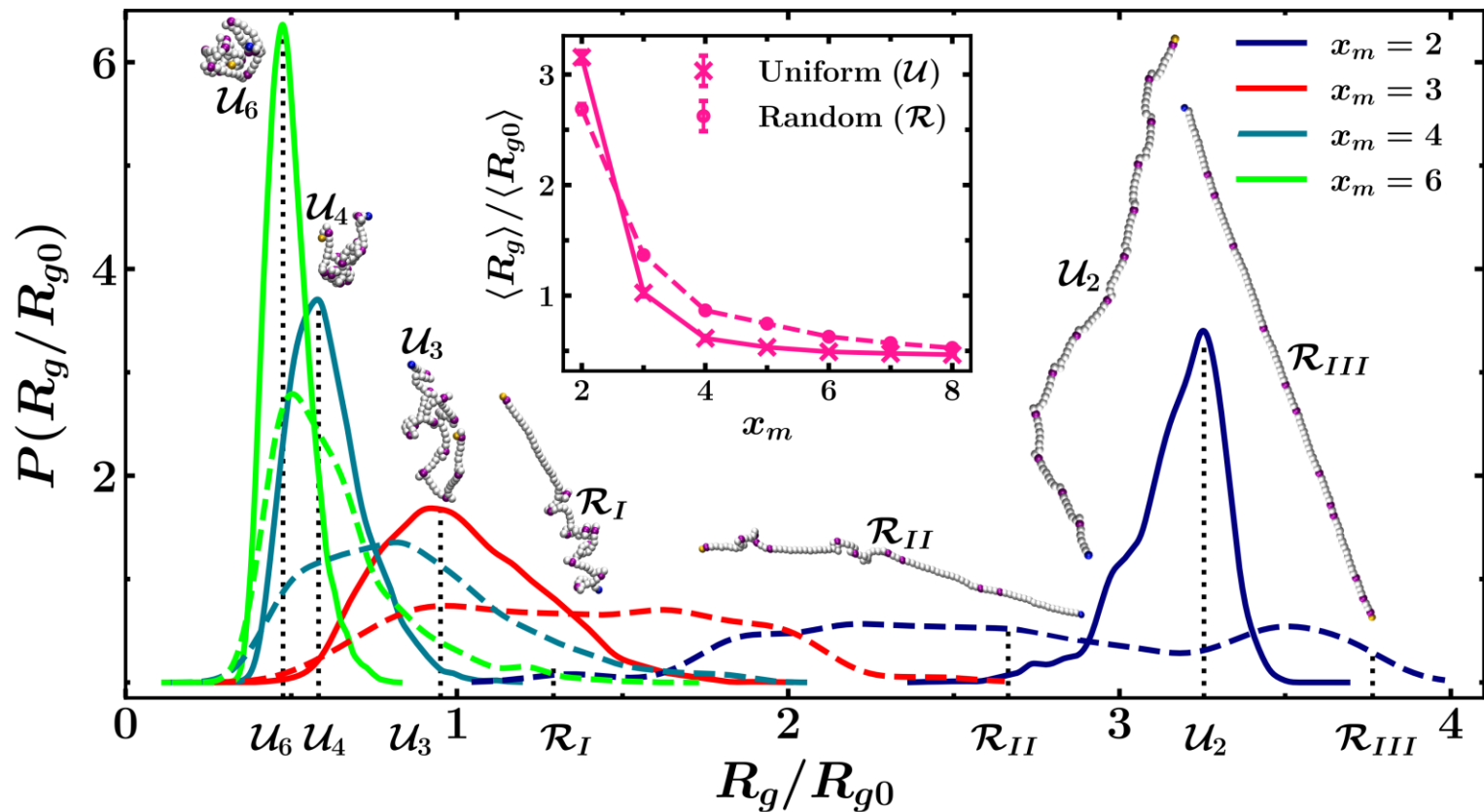
x_m = Position of first motor



How the motors are distributed along the chain is also crucial

Distribution of motors for a fixed motor density

x_m = Position of first motor



- Having passive monomer in front, makes the head loose its directionality, and hence coiled state
- Plethora of possible conformations widens the R_g distribution for the random distribution as compared to the uniform

Summary

- Chemically active flexible linear polymer exhibits a coil-to-globule transition
- While in principle phoresis is a solvent-induced phenomena, our method treats the phoretic thrust as an effective interaction between monomer beads and highlights the effect of HI
- Polar active polymers possess very rich structural and dynamical properties
- The position and activity of the active segment play a dominant role in



Thank you