Migration of active rings in porous media

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Inspired by how the shape deformations in active organisms help them to migrate through disordered porous environments, we simulate active ring polymers in two-dimensional random porous media. Flexible and inextensible active ring polymers navigate smoothly through the disordered media. In contrast, semiflexible rings undergo transient trapping inside the pore space; the degree of trapping is inversely correlated with the increase in activity. We discover that flexible rings swell while inextensible and semiflexible rings monotonically shrink upon increasing the activity. Together, our findings identify the optimal migration of active ring polymers through porous media.

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I. INTRODUCTION

Active agents live and move through the disordered porous environment. The pores serve as selective-permeability barriers in regulating diffusive transport that play a crucial role in tissue protection and cell functioning of human and animal bodies [1-9]. At the cellular level, when a cell touches a permissive surface, it will form adhesive structures to cope with the hostile environments [10-14]. This type of adaptive migration has been observed in different types of cells: amoebae [15,16], neutrophils, bacterial cells [17], and dendritic cells [18,19]. In bioremediation, microscopic organisms migrate through the porous media such as soil and sediments to remove or neutralize the environmental pollutants by metabolic processes [20–22]. The physical properties of the microenvironment play a significant role in the migration of these living objects across all sizes starting from single cells-substrate stiffness and pore size regulate the migration of eukaryotic cells [23-28]-to multicellular organismsnematodes swim in low-viscosity fluids whereas they navigate by crawling on soft surfaces [29,30]. To migrate effectively through crowded disordered environments, cells deform their shapes [31–35] by consuming energy from ATP hydrolysis in two ways; by the action of myosin molecular motors on actin filaments [36-38] or by a propulsive mechanism using the plasma membrane blebs [39]. Hence investigating the mechanism behind the migration of these active agents through the complex porous environments will help us to understand the fundamental physiological and pathological processes.

In unconfined liquid media, a single active particle exhibits transient superdiffusion followed by a long-time enhanced diffusion [40,41]. However, novel nonequilibrium effects emerge in the conformational and dynamical properties of

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a chain of interlinked active particles. For flexible active polymers, the polymer chain swells with increasing activity [42–45]. In contrast, semiflexible active polymers shrink at low activity and swell for large activity [46]. However, much less explored is how the topology of the porous media affects the migration of active agents [47]. Studies of linear active polymers in a two-dimensional periodic porous medium demonstrated that the stiff chains are able to move almost unhindered through the ordered porous medium, whereas the flexible one gets stuck [48]. In biological systems, cell morphology can have a crucial impact on different modes of migration in porous environments. Recent studies have shown that the microconfinement of the porous medium dramatically alters the run-and-tumble motion of rod-shaped bacterial cells to hopping and trapping motion [49,50]. On the other hand, the amoeboid cells, which are typically roundish, are known to migrate fast and adapt quickly to their surroundings [31]. Thus, an active ring polymer can also be a model for mammalian cells [51,52]. Dynamical and conformational properties of active ring polymers in complex environments remain largely elusive and could be markedly different from active linear polymer counterparts despite having an equal number of active monomers in both cases [53,54]. But there have been no systematic studies of such an active ring polymer in random porous environments.

In this work, we explore the dynamics of active ring polymers in two-dimensional random porous media. We extensively analyze the dynamical and conformational properties of the active ring polymer by following the position (r_c) of the center of mass (COM) and the radius of gyration (R_g) . In general, we find that the dynamics of the COM of the ring polymer in porous environment is always enhanced due to the combined effects of activity and conformational fluctuations of the polymer. Interestingly, the semiflexible ring polymer shows a transition from a trapped state to escaping with increasing activity at longer times, whereas such trapping events are absent in the case of flexible ring polymers.

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FIG. 1. (a) A snapshot of active ring polymer in porous media and the schematic sketch of active ring polymer. Polymer is regarded as beads connected by springs. (b) A representative trajectory of the active ring polymer in the porous medium. The magenta arrows represent ring conformations corresponding to different frames in the trajectory.

Moreover, upon increasing activity, the distribution of R_g begins to broaden towards larger values of R_g indicating that the activity drives the flexible ring polymers to continuously swell. However, for the inextensible and semiflexible ring polymers, the distribution of R_g broadens and shifts towards lower values of R_g as a function of activity. This is indicative of shrinking of the active ring polymer. As a comparative study, the pore size effect is also specifically investigated. Hence, studies of active ring polymers in porous environments will help in designing the active migration strategies of shapedeforming systems.

II. METHOD

A. Model and simulation details

We model the polymer ring as a sequence of N selfpropelled beads of diameter σ connected by N finitely extensible springs [Fig. 1(a)]. The dynamics of the ring polymer is determined by the evolution of the self-propelled beads of positions r_i , which we simulate using Langevin dynamics,

$$m\frac{d^{2}\mathbf{r}_{i}(t)}{dt^{2}} = -\gamma \frac{d\mathbf{r}_{i}}{dt} - \sum_{j} \nabla V(\mathbf{r}_{i} - \mathbf{r}_{j}) + \mathbf{f}_{i}(t) + \mathbf{F}_{a,i}(t),$$
(1)

where the drag force, $\gamma \frac{d\mathbf{r}_i}{dt}$, is the velocity of each bead times the friction coefficient γ , *m* is the mass of monomer, V(r) is the total interaction potential which gives rise to the conservative forces, thermal force $\mathbf{f}_i(\mathbf{t})$ is modeled as Gaussian white noise with zero mean and variance $\langle f_i(t')f_j(t'')\rangle =$ $4\gamma k_B T \delta_{ij} \delta(t' - t'')$, and $\mathbf{F}_{a,i}(t)$ is the active force which drives the system out of equilibrium. $\mathbf{F}_{a,i}(t)$ has the magnitude F_a , acts along the unit vector [40] of each *i*th monomer, $\mathbf{n}(\theta_i) =$ $(\cos \theta_i, \sin \theta_i)$, where θ_i evolves as $\frac{d\theta_i}{dt} = \sqrt{2D_R} \mathbf{f}_i^R$, D_R is the rotational diffusion coefficient, and \mathbf{f}_i^R is the Gaussian random number with a zero mean and unit variance. Hence, the persistence time of the individual monomers is related to the rotational diffusion coefficient, D_R , as $\tau_R = \frac{1}{D_R}$. We measure the distance in units of the diameter of the monomers of the ring polymer σ , energy in k_BT , and time in $\tau = \sqrt{\frac{m\sigma^2}{k_BT}}$. The total interaction potential $V(r) = V_{\text{FENE}} + V_{\text{BEND}} + V_{\text{WCA}}$ consists of bond, bending, and excluded volume contributions. The bond stretching is controlled by a FENE potential:

$$V_{\text{FENE}}(r_{ij}) = \begin{cases} -\frac{kr_{\text{max}}^2}{2} \ln\left[1 - \left(\frac{r_{ij}}{r_{\text{max}}}\right)^2\right], & \text{if } r_{ij} \leqslant r_{\text{max}} \\ \infty, & \text{otherwise.} \end{cases}$$
(2)

where r_{ij} is the distance between two neighboring monomers in the ring polymer with a maximum extension of $r_{max} = 1.5\sigma$, and k is the spring constant [55]. To achieve the condition of inextensibility, k is set very high for the inextensible ring polymer (k = 1000). The stiffness of the ring polymer is implemented through the bending potential,

$$V_{\text{BEND}}(\phi_i) = \kappa (1 - \cos \phi_i), \qquad (3)$$

where κ is the bending modulus and ϕ_i is the angle between the bond vectors *i* and *i* + 1. To account for self-avoidance a pair of monomers of the ring polymer interact via the repulsive Weeks-Chandler-Andersen (WCA) potential [56]:

$$V_{\text{WCA}}(r_{ij}) = \begin{cases} 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6} \right] + \epsilon, & \text{if } r_{ij} < 2^{1/6} \sigma_{ij} \\ 0, & \text{otherwise,} \end{cases}$$
(4)

where r_{ij} is the separation between the interacting particles, $\epsilon_{ij} = 1$ is the strength of the steric repulsion, and $\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$ determines the effective interaction diameter, with $\sigma_{i(j)}$ being the diameter of the interacting pairs. The porous medium is modeled by randomly placing M (M = 1200, 2000, 2500, 3000) number of particles that are allowed to overlap inside a two-dimensional square box of length 300 σ . The size of the beads forming the porous medium, σ_P , ranges from 1 to 10 σ , and the size distribution of these particles falls under a Gaussian distribution of mean 6σ . These beads are static throughout the simulations and interact with the monomers of the ring polymer through the WCA potential [Eq. (4)]. We have considered three different cases: flexible (k = 30 and $\kappa = 0$), inextensible (k = 1000 and $\kappa = 0$), and semiflexible (k = 30 and $\kappa = 1000$) ring polymers in the porous media.

All simulations are performed using the Langevin thermostat, and the equation of motion is integrated using the velocity Verlet algorithm in each time step. We initialize the system by randomly placing the ring polymers inside the porous medium and relaxing the initial configuration for 2×10^6 steps. All production simulations are carried out for 10^9 steps where the integration time step is considered to be 10^{-5} and the positions of the monomers are recorded every 100 steps. The simulations are carried out using LAMMPS [57], a freely available open-source molecular dynamics package.

B. Characterization of the porous media

We characterize the pore space structure with the average pore size ξ . We place passive tracer particles at different random locations in the media and allow them to diffuse through the polydisperse porous media. The average pore size ξ is calculated from the time-and-ensemble averaged meansquare displacements (MSD) of the passive tracer particle in



FIG. 2. Log-log plot of $\langle \overline{\Delta r^2(\tau)} \rangle$ vs τ of the passive tracer particle in different porous media.

the porous medium (Fig. 2). At a longer time, the tracer is confined by the obstacles, and the MSD saturates. Then we

take the square root of this saturated value and add the tracer particle diameter to get ξ . The values of ξ obtained from different tracer trajectories are binned to construct a histogram from which the ensemble-averaged probability distribution of ξ , $P(\xi)$, is computed (Fig. S1 [58]). To change the average pore size, ξ , we increase the obstacle density by adding particles, keeping the same width of the Gaussian distribution of the sizes of the obstacles. The pore sizes of these different porous media are less than, bigger than, or comparable to the average R_g of the passive ring polymer in unconfined space.

III. RESULTS

We first investigate the dynamics of flexible ring polymers ($\kappa = 0$) with a small spring constant of k = 30 to find that active motion drives instantaneous deformations in the polymer rings; tracking the center of mass (r_c) of each ring reveals that the optimal motility of these rings is facilitated by a series of conformational changes [Fig. 1(b) and Movie



FIG. 3. The COM trajectory, log-log plot of $\langle \Delta r_c^2(\tau) \rangle$ vs τ , and log-linear plot of $\alpha(\tau)$ vs τ of the ring subjected to different F_a for flexible [(a), (b), and (c)], inextensible [(d), (e), and (f)], and semiflexible [(g), (h), and (i)] ring polymers, respectively, in the porous medium with $\xi = 6.92$. For each time interval τ , the error bars corresponding to standard deviation are plotted, even if too small to be visible. N is the number of monomers of the ring polymer and R_g^0 is the average radius of gyration of the passive ring polymer in unconfined space.

S1 [58]]. To further quantify the dynamical behavior of the active ring polymer, we analyze the time-and-ensemble averaged MSD, $\langle \overline{\Delta r_c^2(\tau)} \rangle$, of the center of mass as a function of lag time τ . First, we compute the time-averaged MSD, $\overline{\Delta r_i^2(\tau)} = \frac{1}{T'-\tau} \int_0^{T'-\tau} [\mathbf{r}_i(t+\tau) - \mathbf{r}_i(t)]^2 dt$ from the time series $\mathbf{r}_i(t)$. Here T' is the total run time and τ is the lag time (width of the window slide along a single trajectory for averaging). To obtain the time-and-ensemble-averaged MSD, we compute the average, $\langle \overline{\Delta r^2(\tau)} \rangle = \frac{1}{N'} \sum_{i=1}^{N'} \overline{\Delta r_i^2(\tau)}$, where N' is the number of independent trajectories. If measured time series are not long enough, $\langle \Delta r^2(\tau) \rangle$ provides smoother curve when N' is sufficiently large. For a given set of parameters we generate 20 independent trajectories of the ring polymer. Typically, $\langle \overline{\Delta r^2(\tau)} \rangle$ scales with τ as $\sim \tau^{\alpha}$, where $\alpha(\tau) = \frac{d \log(\overline{\Delta r^2(\tau)})}{d \log \tau}$. The scaling exponent α determines the type of diffusion: $\alpha = 1$ corresponds to normal diffusion, $\alpha < 1$ corresponds to subdiffusion, and $\alpha > 1$ corresponds to superdiffusion. In the absence of any active force and in an unconfined environment, MSD varies linearly with time reflecting the overdamped dynamics of the ring polymer (Fig. S2 [58]). In unconfined space, the MSD of the ring polymers exhibits three distinct regimes of motion in the presence of activity: a short-time thermal diffusion, intermediate superdiffusion, and enhanced diffusion at longer times as compared to the passive polymers [31,42,44,46,59-61]. The intermediate superdiffusion occurs at an earlier time with an increase in the activity. A similar trend in the translational dynamics of the center of mass is observed in analytical studies of an ideal free active linear polymer [42,60] and ring polymer [62] where the activity is modeled as an Ornstein-Uhlenbeck process.

A. Migration of flexible, inextensible, and semiflexible rings in the porous media: Smooth migration vs trapping

To further investigate the dynamics of the rings under confinement, we simulate motions of an active ring polymer inside disordered polydisperse porous media modeled by randomly placing M number of circular obstacles that are allowed to overlap inside a two-dimensional square box of fixed size. The size of the obstacles forming the porous media follow Gaussian distribution. These obstacles are static throughout the simulations and interact with the monomers of the ring polymer via the repulsive Weeks-Chandler-Andersen (WCA) potential [56]. Different porous media with varying void volumes are prepared by varying the number of obstacles M (M = 1200, 2000, 2500, 3000). We characterize the extent of confinement offered by these porous media by the average pore size, ξ , measured for each porous medium by identifying the average cage size for a thermal fluctuating tracer (Fig. 2). Together, these measurements indicate the variation in the extent of confinement. We carry out independent simulations by randomly placing the ring polymer inside the pore space.

In a disordered environment, the dynamics of the flexible ring polymers is altered and is set by the overall activity and the extent of confinement [Fig. 3(a) and Movie S2 [58]]. Primarily, a transient behavior between two regimes of motion emerges: a short-time superdiffusion which occurs due to active motion, and a long-time diffusive behavior [Figs. 3(b) and 3(c)]. However, in the case of inextensible rings (k =



FIG. 4. The effective translational diffusion coefficient $(D_T^{F_a})$ of the flexible and inextensible ring polymers (N = 50) subjected to different activity in porous medium with $\xi = 6.92$.

1000, $\kappa = 0$) an intermediate subdiffusive behavior emerges for passive and lower activities followed by the diffusive behavior at long time [Figs. 3(d)-3(f)]. The rings get caged intermittently (Movie S3 [58]). We extract the values of effective translational diffusion coefficients $(D_T^{F_a})$ of the flexible and inextensible active ring polymers by fitting the long-time $\langle \overline{\Delta r_c^2(\tau)} \rangle$ with $4D_T^{F_a}\tau$. In Fig. 4 we plot $D_T^{F_a}$ as a function of F_a . The diffusivity of the rings increases with increasing activity in the porous medium and for the inextensible ring polymer has a larger diffusivity as compared to the flexible ring for a fixed F_a . This implies that the activity always helps the ring polymers to navigate more efficiently through the porous media. Finally, we investigate the dynamics of semiflexible ring polymers ($\kappa = 1000$) with a small spring constant of k = 30. The high bending rigidity restricts the conformational fluctuations leading to the trapping of these ring polymers in tight spaces of the porous environment [Fig. 3(g)]. For small activities, long-time subdiffusive behavior is more pronounced in the dynamics of the semiflexible rings [Figs. 3(h) and 3(i)]. However, an increase in activity enhances the conformational fluctuations of the semiflexible ring polymers, which helps them to escape from the microconfinements of the porous medium (Movie S4 [58]). This behavior is illustrated in Fig. 3(g) where for constant F_a , the path traversed by the COM of a semiflexible ring polymer is reduced compared to that of the flexible and inextensible rings. We find that the dynamical behavior of the flexible ring polymer as observed in Fig. 3(a) persists for a broad range of ξ , but becomes rather enhanced for higher ξ as exemplified by the different trajectories in Figs. S3(a) and S3(b) [58]. At the short and intermediate times, $\alpha(\tau)$ remains independent of the porous structure of the environment [Fig. S3(c) [58]]. At longer time, $\alpha(\tau)$ exhibits an increase with ξ indicating the polymer exploring different random pores in the medium.

B. Conformations of rings in unconfined and porous media: Activity-induced swelling and shrinking

To elucidate the subdiffusive dynamics, we consider the effect of activity on the conformations of ring polymers. In this regard, we compute the probability distribution of radius of gyration, $P(R_g)$ as a function of F_a and ξ . For a polymer,



FIG. 5. $P(R_g)$ vs R_g for flexible [(a), (d)], inextensible [(b), (e)], and semiflexible [(c), (f)] ring polymers (N = 50) subjected to different activity in the unconfined space and porous medium with $\xi = 6.92$, respectively.

the radius of gyration is defined as

$$R_g = \sqrt{\frac{1}{N} \sum_{i=1}^{N} m(r_i - r_{\rm com})^2},$$
 (5)

where N is the total number of monomers of the ring polymer, and $r_{\rm com}$ is the center of mass position. R_g is calculated at each time step of every simulation after the system reaches the steady state. Then a single trajectory is created by stitching different individual trajectories. This single trajectory is binned to construct a histogram from which the ensembleaveraged probability distribution of R_g is computed. In an unconfined environment, increasing activity leads to constant swelling of the flexible ring polymer, and hence the peaks of $P(R_g)$ shift to larger R_g with F_a [Fig. 5(a)]. The reason for the swelling is an increase in the stretching of the chain due to activity by effectively pulling it from different directions. For inextensible ring polymers, there is no shift in the peak values of $P(R_g)$ because the bond fluctuations of the chain are restricted by the very high value of a spring constant in the unconfined space [Fig. 5(b)]. For a semiflexible ring polymer also, we find that the peaks of $P(R_g)$ are almost independent of F_a for the wide range of activities in unconfined space [Fig. 5(c) and Fig. S4(a) [58]]. This implies, for the very high value of bending potential, that the bending rigidity dominates over the activity. In contrast to the unconfined space, the flexible ring polymer continuously swells with increasing F_a even inside the porous medium [Fig. 5(d)], but $\langle R_{\rho} \rangle$ is smaller as compared to the unconfined space (Fig. S5 [58]). In the unconfined space, the ring can freely change its conformations, while inside the tight pore, the conformational changes are restricted by the obstacles in the media due to limited space

available within the obstacles forming the pore confinements. Interestingly, for the inextensible ring polymers, not only does the swelling cease, but also an opposite behavior is observed in the porous medium. The peaks of the distributions shift towards smaller values of R_g with an increase in F_a , implying the activity-induced shrinking of the ring in the porous medium [Fig. 5(e) and Fig. S4(b) [58]]. However, a recent study showed that a single active linear polymer undergoes a coil-to-globule-like transition in free space [63]. It is important to note that, in their model, active force is applied along the backbone of the chain which pushes the filament along the bond directions and leads to shrinking. In our system, the mechanism of activity-induced shrinking is quite different. In the pore confinement, the ring polymer with higher activity more frequently collides with the obstacles with a larger effective force. This subsequently generates more fluctuations along the inward transverse direction of the contour responsible for the shrinking of ring polymer. The semiflexible ring polymer also exhibits similar features of $P(R_{g})$ as inextensible ring polymers [Fig. 5(f)]. The activity-induced inward transverse fluctuations attempt to crumple the ringlike structure in the case of inextensible and semiflexible ring polymers. However, this is opposed by the high bending rigidity of the ring polymers when the bending potential is very high. Thus, bending rigidity reduces the extent of shrinking of the semiflexible ring polymer compared to the inextensible ring polymer [Fig. S5(b) [58]]. We calculate the time autocorrelation functions of R_g , $C_{R_g}(\tau) = \frac{\langle \overline{R_g^2(t)R_g^2(t+\tau)} \rangle - \langle \overline{R_g^2(t)} \rangle^2}{\langle \overline{R_g^4(t)} \rangle - \langle \overline{R_g^2(t)} \rangle^2}$ to investigate the conformational relaxation of the ring polymer in porous media [64]. For a flexible ring, $C_{R_a}(\tau)$ increases with activity, whereas it decreases for the inextensible and semiflexible rings (Fig. 6). Hence, the trends in $C_{R_e}(\tau)$ support the



FIG. 6. $\langle C_{R_g}(\tau) \rangle$ vs τ for flexible (a), inextensible (b), and semiflexible (c) ring polymers (N = 50) subjected to different activity in the porous medium with $\xi = 6.92$.

swelling of the flexible ring and shrinking of the inextensible and semiflexible rings in the porous media. We also plot 1 – $\text{CDF}(R_g)$ corresponding to each distribution of $P(R_g)$, where $\text{CDF}(R_g) = \frac{\sum_{0}^{R_g} P(R_g) R_g}{\sum_{0}^{\infty} P(R_g) R_g}$ is the cumulative distribution function of R_g (Fig. S6 [58]). 1 – $\text{CDF}(R_g)$ qualitatively demonstrates the similar behavior as observed in $P(R_g)$.

trapping of the semiflexible ring and the smooth migration of the flexible ring polymer in porous media are not solely determined by the pore confinement. It depends on the nature of the rings. The conformational properties are qualitatively similar to Figs. 5(d) and 5(f) even for a flexible ring of size comparable to the pore size and a semiflexible ring of size smaller than the pore size [Figs. 7(d) and 7(h)].

IV. DISCUSSION

C. Nature of the ring determines the migration in the porous media

Next, we compare the dynamical and conformational properties of active rings in a different fashion. We consider two different cases: a flexible ring of size comparable to the pore size and a semiflexible ring of size smaller than the pore size. The trapping of the semiflexible ring is observed even when the ring is smaller than the pore size [Figs. 7(a)-7(c)]. However, in the case of the flexible polymer, the ring moves from one pore to another smoothly even if the ring size is comparable to the pore size [Figs. 7(e)-7(g)]. Hence the Our simulations characterize how the motion of an active ring polymer in porous media is regulated by both pore-scale confinement and the individual bead's activity. The dynamics of the COM of a ring polymer is enhanced by orders of magnitude and exhibits an intermediate superdiffusive behavior in the presence of activity as compared to the passive ring. Moreover, the semiflexible ring polymer displays a transition from trapping at small activities to escaping at higher activities due to its stretched conformations. According to analysis, the ring polymer shows distinct conformational changes at low



FIG. 7. The COM trajectory, log-log plot of $\langle \overline{\Delta r_c^2(\tau)} \rangle$ vs τ , log-linear plot of $\alpha(\tau)$ vs τ , and $P(R_g)$ vs R_g of the ring subjected to different F_a for flexible (N = 100) [(a), (b), (c), and (d)] and semiflexible (N = 50) [(e), (f), (g), and (h)] ring polymers in the porous medium with $\xi = 6.92$ and 9.84, respectively. For each time interval τ , the error bars corresponding to standard deviation are plotted in $\langle \overline{\Delta r_c^2(\tau)} \rangle$ [(b), (f)] and $\alpha(\tau)$ [(c), (g)], even if too small to be visible.

and high spring constants in porous environments. Crowders of the porous media induce an unavoidable collapse of the passive ring polymer. However, the activity exerts a force on the bonds attempting to stretch the ring polymers. Hence, upon increasing the activity, the flexible ring polymer swells, while the inextensible ring polymer collapses. The conformational restrictions by a higher spring constant increase the inward transverse fluctuations leading to shrinkage of the ring polymer with increasing activity. A semiflexible active ring polymer also suffers an activity-induced collapse but with a larger average size due to its extended confirmations as compared to the inextensible active ring polymer.

The physics underlying the phenomena we report here relies on the motion of a ring polymer driven by the active fluctuations in porous environment. In our model, superdiffusive behavior arises at an intermediate time due to the activity driven breakdown of the fluctuation-dissipation the-

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orem. However, superdiffusive behavior can also occur in a collection of passive elastic ring polymers due to the interplay between the particle deformations and dynamic heterogeneity [65]. Hence, further studies of collective migration of active ring polymers in complex environments with the inclusion of softness in the monomers [65] are anticipated in the future.

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