

Friction of two-dimensional colloidal particles with magnetic dipole and Lennard–Jones interactions: A numerical study

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Abstract: We use Langevin simulations to study the sliding friction of two-dimensional colloidal particles on a substrate with randomly distributed point-like pinning centers. The colloidal particles are modeled to interact with each other through repulsive magnetic dipole and attractive Lennard–Jones potentials. The subsequent occurrence of superlubricity, wherein the average friction force equals to zero, is accompanied by the appearance of islands with clear boundaries in the microscopic colloidal structures for weak pinning substrates. Friction arises for strong pinning substrates, and the average friction force increases with the substrate pinning intensity, and further, the islands disperse into disordered plastic structures. Moreover, the average friction force decreases with the repulsion intensity between the colloidal particles, and superlubricity finally results when the repulsion becomes sufficiently strong. Superlubricity also occurs for sufficiently weak attraction between colloidal particles, with an increase in the attraction intensity between colloidal particles leading to a nonlinear increase in the average friction force. With increasing temperature, the average friction force firstly increases and subsequently decreases rapidly. The above results can provide a theoretical framework for biological self-organization via utilization of the friction properties of microscopic or mesoscopic colloidal systems.

Keywords: friction; sliding friction; superlubricity; self-assembly

1 Introduction

Friction plays a central role in various systems that range from the nanometer to geophysical scales [1]. Friction is encountered in all aspects of science and technology, and this has led to continual advancements in friction studies over centuries. In this context, developments in nanotechnology permit the study of friction at the nano/micro scales, and studies of nano-friction can provide greater insights into the microscopic nature of friction [1–3].

Meanwhile, colloidal suspensions provide unique possibilities for obtaining mesoscopic information about nature, for, e.g., mesoscopic friction behaviors, because the size of colloidal particles lies in the range between nanometers and micrometers. Some colloidal particles are superparamagnetic, and the magnitude

of the induced magnetic moment in these colloidal particles scales linearly with the applied magnetic field strength [4–8]. Thus, the interaction between magnetized colloidal particles has the form of a repulsive magnetic dipole potential. Here, we note that magnetic gels can be easily prepared [9] for use in experiments, and the dynamic properties of magnetized colloids are more abundant than those of charged colloids [10–13], for, e.g., there are richer dynamic phase transitions near depinning in the magnetized colloids [13]. In this study, we focus on magnetized colloids.

Recently, active colloids have attracted considerable research interest. Active systems can actively absorb energy from the environment and overcome resistance (i.e., energy barrier) through energy storage [14], as in the case of bacterial colonies of fish and birds and tissues of cells; such systems are different from passive

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systems that acquire energy from the surrounding environment and subsequently restore energy to the environment. It is known that the abovementioned activity originates from weak attractive interactions between individuals in the systems [15–20], for, e.g., van der Waals interaction between colloidal particles. Such self-propelling interactions between individual members of active systems [21] drive the systems to non-equilibrium states, which leads the systems exhibiting a series of novel behaviors that cannot be observed under equilibrium [20–25]. The most striking behaviors include the formations of clusters with finite size or islands with clear boundaries (the so-called living islands) [20–25]. These structures are closely related to biological self-organization [17, 20–25]; in this context, we note that biological activity is also one of the remarkable characteristics of biotribological problems in relation to general tribological problems.

Currently, nanotribology studies are seeking to explore novel routes, for, e.g., phase transitions [26], to achieve frictional control, which can in turn be used to control biological activity and self-organization [1]. Against this backdrop, here, we numerically investigate the sliding friction of two-dimensional (2D) active magnetized colloids on a substrate with randomly distributed point-like pinning centers. The substrate is a realistic quenched one, which is different from an ordered substrate [27]. The active magnetized colloidal particles are modeled as interacting with each other via repulsive magnetic dipole and attractive Lennard–Jones potentials [20, 28]. We attempt to determine the relationship between sliding friction and dynamic phases and phase transitions, which can provide a theoretical framework for the control of biological self-organization via utilization of the friction properties of mesoscopic colloidal systems.

2 Model

The system of interest consists of 400 active magnetized colloidal particles, which are modeled to interact with each other through repulsive magnetic dipole and attractive Lennard–Jones potentials. These particles are initially placed in an ideal triangular lattice satisfying periodic boundary conditions. The substrate is simulated by 400 randomly distributed point-like pinning centers. We describe the motion of colloidal

particles by means of the Langevin equation [11–13, 17, 20, 28, 29]:

$$\eta \frac{d\mathbf{R}_i}{dt} = -\sum_{i \neq j} \nabla_i U_{cc}(\mathbf{R}_i - \mathbf{R}_j) - \sum_{j'} \nabla_i U_{cp}(\mathbf{R}_i - \mathbf{r}_{j'}) + \mathbf{F}_i^T \quad (1)$$

where η is the viscosity coefficient, and \mathbf{R}_i and $\mathbf{r}_{j'}$ are the positions of the i -th colloidal particle and j' -th pinning center, respectively. Further, $U_{cc}(r)$ with $r = |\mathbf{R}_i - \mathbf{R}_j|$ is the interaction between colloidal particles, including the repulsive component $U_{cc}^{\text{rep}}(r)$ and attractive component $U_{cc}^{\text{att}}(r)$. Further, $U_{cp}(r')$ with $r' = |\mathbf{R}_i - \mathbf{r}_{j'}|$ is the interaction between the colloidal particles and pinning centers in the substrate. \mathbf{F}_i^T is the thermal force.

When a magnetic field \mathbf{B} acts perpendicular to the plane of the system, the induced magnetic dipole potential has the repulsive form [10, 11–13, 20, 28, 29]:

$$U_{cc}^{\text{rep}}(r) = \frac{A_v^2}{r^3} \quad (2)$$

where $A_v = \sqrt{\frac{\mu_0}{4\pi}} \chi B$, with μ_0 being the vacuum permeability, χ being the magnetic susceptibility, and B being the magnetic field strength. Further, A_v is the repulsion intensity between colloidal particles, and it is controlled completely by the magnetic field strength B .

The attractive interaction $U_{cc}^{\text{att}}(r)$ is chosen as the Lennard–Jones potential [16, 20, 24, 28]:

$$U_{cc}^{\text{att}}(r) = 4A_e \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (3)$$

Here, A_e and σ are the attraction intensity and diameter of the colloidal particles, respectively.

Next, we choose the interaction between colloidal particles and pinning centers in the substrate, $U_{cp}(r')$, as the traditional Gaussian attractive potential [11–13, 20, 28, 29]:

$$U_{cp}(r') = -A_p e^{-\left(\frac{r'}{r_p} \right)^2} \quad (4)$$

where A_p is the substrate pinning intensity, r_p is the radius of the pinning center, and we assume $r_p = 0.2a_0$,

with a_0 being the lattice constant of the ideal triangular lattice.

The thermal force F_i^T describes the coupling process with a heat bath and satisfies [11–13, 20, 28, 29]:

$$\langle F_i^T(t) \rangle = 0 \quad (5)$$

and

$$\langle F_{i\alpha}^T(t) F_{j\beta}^T(t') \rangle = 2\eta T \delta_{ij} \delta_{\alpha\beta} \delta(t-t') \quad (6)$$

where subscripts α and β are the components of F_i^T and F_j^T , respectively. Further, T is the temperature of system.

We present all quantities in dimensionless units in our simulations. The length is based on the lattice constant a_0 , and we scale the temperature with respect to the bare Kosterlitz–Thouless melting temperature of a pure system, T_{m0} [30]. The time scale is chosen as $T_{m0}/\eta a_0^2$. We measure the average friction force as [1, 27]:

$$F_L = -\eta v \quad (7)$$

with v being the average colloidal velocity along the x symmetric axis. Further, $\Delta t = 0.001$ is set as the time integration step, and the averages are evaluated over 2×10^5 steps after setting 1×10^5 steps for equilibrium.

3 Results and discussion

3.1 Zero-temperature case

Firstly, we investigate the influence of the substrate pinning intensity on the average friction force. Given a low repulsion intensity ($A_v = 0.1$) and a high attraction intensity ($A_e = 1000$), we present the pinning intensity (A_p) dependence of the average friction force F_L in Fig. 1, from which we can clearly infer the superlubricity phenomenon, i.e., $F_L \approx 0$, over a large range of values of A_p ($A_p < 4$). Islands with clear boundaries (i.e., living islands [16]) and separation between different islands are observed in the microscopic structures of colloidal particles for sufficiently weak pinning substrates ($A_p \leq 0.1$), as shown in Fig. 2(a), where the attraction between colloidal particles is dominant and all the colloidal particles are organized

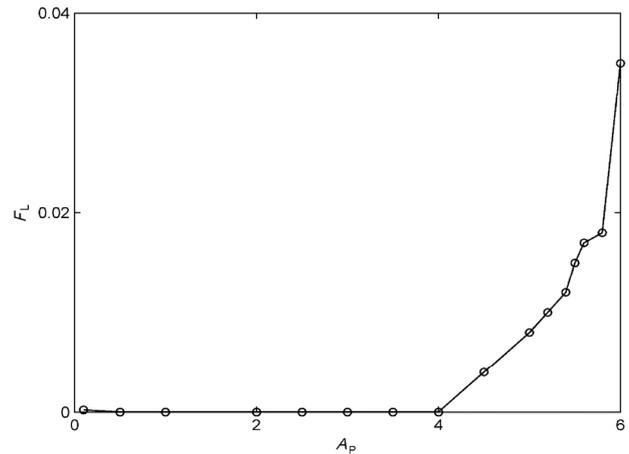


Fig. 1 Dependence of average friction force on substrate pinning intensity.

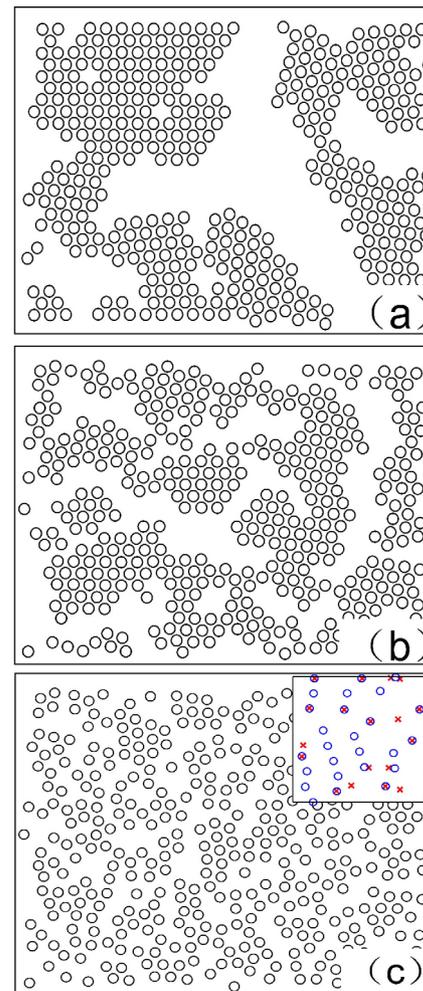


Fig. 2 Coordinates of colloidal particles for (a) $A_p = 0.1$, (b) 0.5, and (c) 5. The inset of (c) shows a snapshot of (c), with the substrate pinning centers denoted by crosses, and free colloidal particles are clearly visible in the channels within different pinning centers.

into living islands. With increase in the pinning intensity ($0.1 < A_p \leq 4$), the attraction between colloidal particles and pinning centers in the substrate becomes comparable with the attraction between colloidal particles, and the living islands are dispersed, as shown in Fig. 2(b). In such a case, there is no free particle in the channels within different pinning centers and the superlubricity is still maintained.

As A_p is further increased ($A_p > 4$), the attraction between colloidal particles and pinning centers in the substrate overcomes the attraction between colloidal particles, and the island structures are destroyed, as shown in Fig. 2(c). Some colloidal particles escape from the islands and lie in the channels within different pinning centers, thus leading to the occurrence of friction. Parameter F_L firstly exhibits a basic linear increase and subsequently increases rapidly when A_p is increased to ~ 6 , as shown in Fig. 1.

Next, we examine the influence of the repulsion intensity between colloidal particles on the sliding friction. For a large pinning intensity ($A_p = 5$) and a large attraction intensity between colloidal particles ($A_c = 1000$), the repulsion intensity (A_v) dependence of the average friction force F_L is presented in Fig. 3. We observe friction for sufficiently small values of A_v , and the colloidal particles are in the destroyed island structures, as shown in Fig. 4(a). In such a case, the repulsion between colloidal particles is so small that it can be neglected, and the attraction between colloidal particles and substrate pinning centers becomes comparable with the attraction between colloidal particles, thereby resulting in some colloidal particles

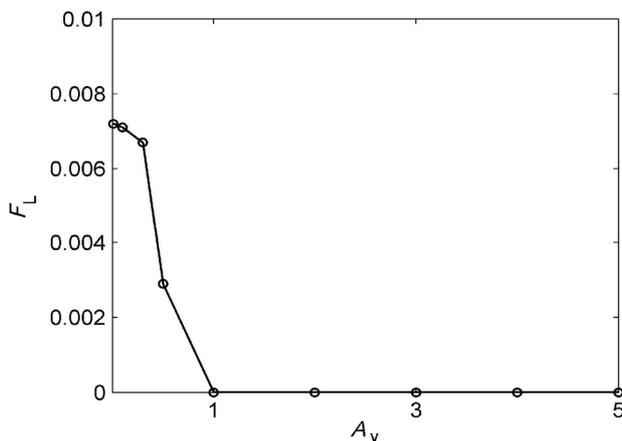


Fig. 3 Dependence of average friction force on repulsion intensity.

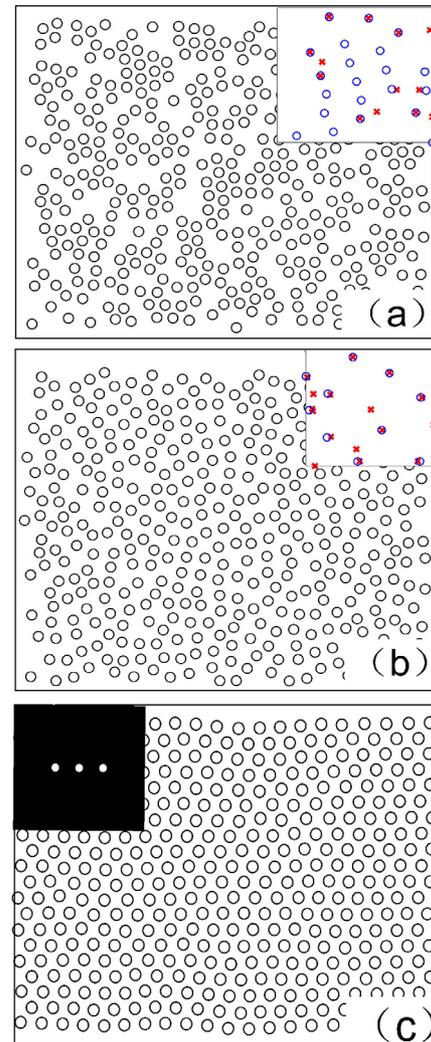


Fig. 4 Coordinates of colloidal particles for (a) $A_v = 0.01$, (b) 1, and (c) 5. The inset of (c) shows its corresponding structure factor defined as $S(\mathbf{k}) = \langle |\frac{1}{N_c} \sum_{i=1}^{N_c} \exp(i\mathbf{k} \cdot \mathbf{R}_i)|^2 \rangle$, where N_c

is the number of colloidal particles. The insets of (a) and (b) show the snapshots of (a) and (b), respectively, with the substrate pinning centers denoted by crosses.

moving within different pinning centers, as shown in the inset of Fig. 4(a).

With increase in A_v , the repulsion between colloidal particles increases, and the colloidal particles in the channels within different pinning centers repulse each other to be close to the pinning centers, causing a decrease in the friction. Superlubricity occurs when there are a few free colloidal particles in the channels within different pinning centers, as shown in the inset of Fig. 4(b), and uniformly plastic structures appear, as shown in Fig. 4(b). A further increase in A_v leads

to $F_L \approx 0$, i.e., superlubricity, and the colloidal particles are in ordered smectic structures, as shown in Fig. 4(c) and its inset, when A_v is increased to be sufficiently large and the repulsion between colloidal particles dominates.

Next, we study the influence of the attraction intensity between colloidal particles on the friction force. Figure 5 presents the attraction intensity (A_e) dependence of the average friction force F_L for $A_p = 5$ and $A_v = 0.1$. Superlubricity occurs over a range of small values of A_e , wherein the colloidal particles assume the form of disordered plastic structures, as shown in Fig. 6(a), and there is no free colloidal particle moving in the channels within different pinning centers, as shown in the inset of Fig. 6(a). As A_e is increased above a certain value (≈ 300), friction arises when the attraction between colloidal particles is comparable with the attraction between colloidal particles and pinning centers in the substrate. As a result, some colloidal particles escape from the pinning centers and move along the channels within different pinning centers, as shown in the inset of Fig. 6(b). Further increasing A_e finally saturates the average friction force F_L to a stable value when the number of colloidal particles within pinning centers remains unchanged, and the colloidal particles are still in form of the disordered plastic structures, as can be observed in Fig. 6(c).

3.2 Finite-temperature case

Finally, we investigate the temperature effect on the sliding friction. The temperature dependence of the average friction force F_L is shown in Fig. 7 for $A_p = 5$

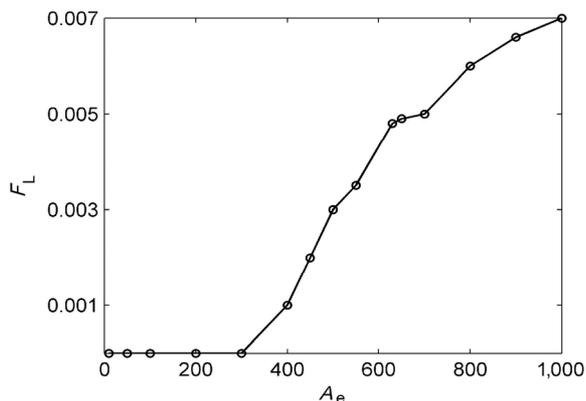


Fig. 5 Dependence of average friction force on attraction intensity.

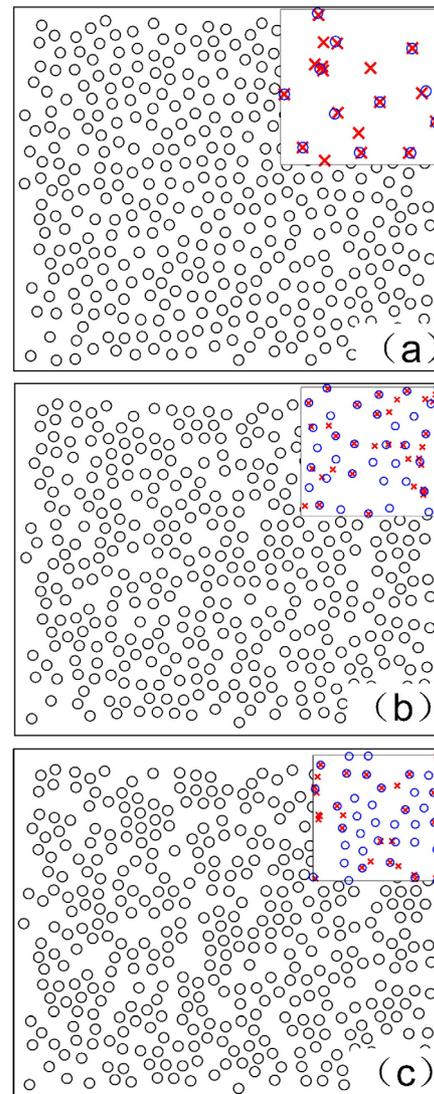


Fig. 6 Coordinates of colloidal particles corresponding to (a) $A_e = 10$, (b) 500, and (c) 1000. The insets of (a), (b), and (c) show the snapshots of (a), (b), and (c), respectively, with the substrate pinning centers denoted by crosses.

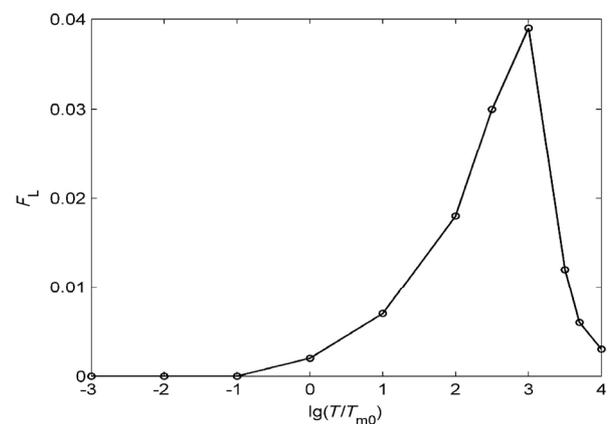


Fig. 7 Dependence of average friction force on temperature.

and $A_e = 1000$. The superlubricity states appear at low temperatures ($T < T_{m0}$) because the thermal fluctuations are so small that they are negligible in relation to the attraction of pinning centers and there are few free colloidal particles moving in the channels within different pinning centers, as shown in the inset of Fig. 8(a).

With increase in the temperature ($T_{m0} < T < 1000T_{m0}$), the thermal fluctuation increases, and some colloidal particles undergo activation to escape from the pinning

centers and move into the channels within different pinning centers, as shown in the inset of Figs. 8(b) and 8(c), thereby leading to the appearance of friction. The number of colloidal particles within different pinning centers increases with the temperature, thus leading to increase in F_L with temperature. However, with further increase in the temperature ($T > 1000T_{m0}$), the thermal fluctuations become so large that the pinning potential is smoothed. This leads to a rapid decrease in the average friction force.

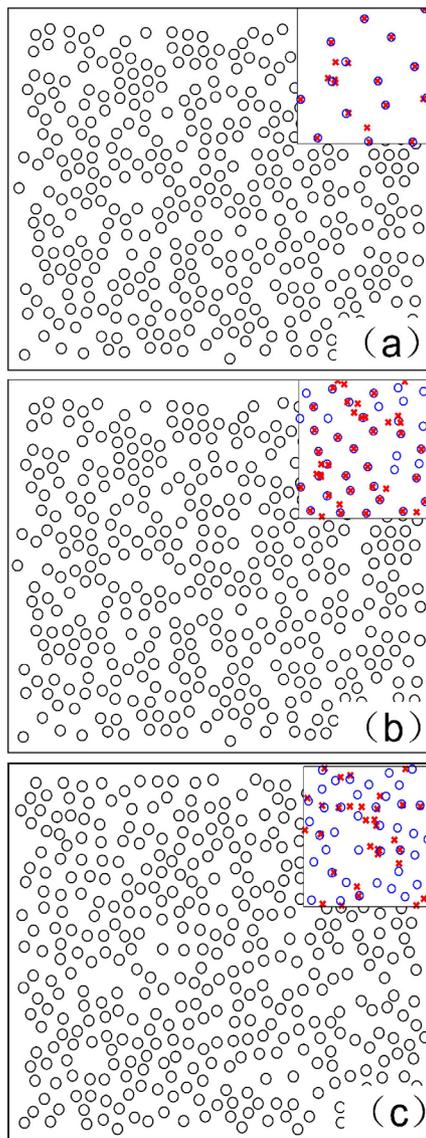


Fig. 8 Coordinates of colloidal particles at different temperatures corresponding to (a) $T = 0.001T_{m0}$, (b) $T = T_{m0}$, and (c) $T = 1000T_{m0}$. The insets of (a), (b), and (c) show the snapshots of (a), (b), and (c), respectively, with the substrate pinning centers denoted by crosses.

4 Conclusions

We numerically investigated the sliding friction behavior of 2D colloidal particles with magnetic dipole and Lennard–Jones interactions on a disordered substrate. At low temperatures ($T < T_{m0}$), the superlubricity phenomenon appears for weak pinning substrates ($A_p < 4$) and weak attraction between colloidal particles ($A_e < 300$) as well as for strong repulsion between colloidal particles ($A_v > 1$). Superlubricity is accompanied by the emergence of islands with clear boundaries in the microscopic colloidal structures for the weak pinning substrates. The observed friction is due to the free colloidal particles moving in the channels within different pinning centers. The average friction force increases nonlinearly with the substrate pinning intensity and the repulsion and attraction intensities between colloidal particles. The thermal fluctuation increases with temperature, thereby leading to an increase in the average friction force below a certain temperature ($T \approx 1000T_{m0}$), above which thermal lubrication takes place and the average friction force decreases rapidly.

Our results are valuable in terms of understanding the mechanism of sliding friction in active mesoscopic particle systems and for controlling biological self-organization by exploiting the friction properties of mesoscopic particle systems.

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