Giant adsorption of microswimmers: duality of shape asymmetry and wall curvature.

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The effect of shape asymmetry of microswimmers on their adsorption capacity at confining channel walls is studied by a simple dumbbell model. For a shape polarity of a forward-swimming cone, the stroke-averaged shape of a sperm, extremely long wall retention times are found, caused by a non-vanishing component of the propulsion force pointing steadily into the wall, which grows exponentially with the self-propulsion velocity and the shape asymmetry. A direct duality relation between shape asymmetry and wall curvature is proposed and verified. Our results are relevant for the design microswimmer with controlled wall-adhesion properties. In addition, we confirm that pressure in active systems is strongly sensitive to the details of the particle-wall interactions.

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Boundaries dominate biological process on all scales. On the microscopic scale, motile organism may bump into various obstacles and boundaries, such as liquid-gas or liquid-liquid interfaces, elastic cell membranes or solid walls. A universal behavior is the accumulation of microswimmers at boundaries. Aside from physico-chemical effects [1], such as van der Waals forces, two main mechanisms have been suggested to explain the wall accumulation, hydrodynamic interactions (HI) [2, 3] and excluded-volume (or steric) forces [4, 5]. The importance of HI on accumulation is still a subject of debate. However, recent experiment in quasi-2D microfluidic channels indicate that surface scattering of sperm and Chlamydomonas at lateral boundaries is dominated by steric forces with multiple flagellar contacts [6, 7], and that HI is almost entirely negligible in such systems, in strong contrast to sperms confined in a 3D channel [8].

Most theoretical studies of simple model swimmers, both in bulk and in confinement, have considered so far cells with a symmetric body shape, in particular, rods [4, 5] or spherical particles [9, 10]. In reality, however, cells usually do not exhibit such high symmetry, and the stroke-averaged shape of sperm or Chlamydomonas rather resembles a forward or a backward swimming cone, respectively [6, 7, 11], see also [12]. This raises the question how a broken for-aft symmetry of the particle shape alters the wall accumulation of cells.

We study this issue by an active Brownian dumbbell model with unequal bead sizes, see Fig. 1. Our simulation results show that swimmers with a sperm-like (polar) shape exhibit huge wall trapping times due to a nonvanishing component of the propulsion force directed steadily toward the wall, thus resulting in a restricted rotational movement. The trapping times increase exponentially with the shape asymmetry and the propulsion strength and could easily, for realistic parameters, exceed the trapping times due to near-field hydrodynamic forces [3, 13, 14]. In contrast, microswimmers with Chlamydomonas-like (antipolar) shape behave similarly to symmetric rod-like particles.

Both in a natural environment and in microfluidic devices [7, 15, 16], microswimmers usually do not swim in straight, but rather in curved or branching microchannels. Therefore, the influence of surface curvature on accumulation of microswimmers [13, 17–21] is of great interest. Based on the analysis of an asymmetric particle near a flat boundary, we found a direct duality relation between the effect of shape asymmetry and surface curvature on accumulation. For example, a polar swimmer close to a flat wall behave similarly to an apolar particle near a concave surface (e.g. a cavity). This is of high relevance for the design microswimmers with controlled wall-adhesion properties.

In order to focus on the effect of the shape asymmetry on the wall accumulation, we model the microswimmer as a self-propelled Brownian dumbbell, and neglect the hydrodynamic interactions with the wall. The dumbbell consists of two spheres with radii $a_1$ and $a_2$ connected by a thin rigid rod of length $l$, see Fig. 1. Its orientation is characterized by a unit vector $\mathbf{e}$ directed along its axis from sphere 2 to sphere 1. The equation of motion for the swimmer’s center is then

$$\dot{r} = V\mathbf{e} + \Xi^{-1}F_w + \eta, \tag{1}$$

where $V$ is the bare propulsion velocity, $\Xi$ is the translational friction tensor, $F_w$ is the steric force due to

FIG. 1. (color online) Sketch of the dumbbell model of asymmetric microswimmers in confinement. The swimmer propel along its instantaneous orientation $\mathbf{e}$ with velocity $V$ in a channel of height $L$. Left: a polar particle ($\theta_0 < 0$); right: an antipolar particle ($\theta_0 > 0$).
swimmer-wall interaction and $\eta$ is a random velocity. The particle is confined in a channel of height $L$ along the $z$-direction. The sphere $\alpha \in \{1,2\}$ interacts with the walls via a screened Coulomb potential $U_\alpha$ [22] with a large inverse screening length $\kappa$ and thus resembles a hard-sphere. The total dumbbell-wall force is $F_w = F_1 + F_2$ with $F_\alpha = -\nabla r_\alpha U_\alpha$ where $r_\alpha$ is the position of sphere $\alpha$. The Gaussian white-noise velocity $\eta$ obeys 
\[
\langle \eta(t)\eta(t') \rangle = 2k_BT\Xi^{-1}\delta(t-t'),
\]
where $k_BT$ is the thermal energy scale and $\Xi = \gamma_||ee + \gamma_\perp(1-ee)$ is the translational friction tensor with the friction coefficients $\gamma_||$ and $\gamma_\perp$ for motions parallel and perpendicular to $e$, respectively. The orientation evolves according to
\[
\dot{\xi} = (T_w/\gamma_r + \xi) \times e,
\]
where $\xi$ is a Gaussian white-noise vector with 
\[
\langle \xi(t)\xi(t') \rangle = 2D_\xi\delta(t-t').
\]
and $D_\xi = k_BT/\gamma_r$ is the rotational diffusion coefficient. The torque due to the wall interaction is $T_w = T_1 + T_2$ with $T_1 = (r_1 - r) \times F_1 = l(e \times F_1)/2$ and $T_2 = -(e \times F_2)/2$. We solve Eqs. (1) and (2) numerically using standard methods [23].

Dimensionless numbers characterising the system are the Peclet number $Pe = V/(lD_r)$, which is the ratio of the swimming persistence length $V/D_r$ to the rod length $l$, and the shape asymmetry parameter $\sin(\theta_0) = (a_1 - a_2)/l$, which is $\sin(\theta_0) < 0$ for polar (sperm-like) and $\sin(\theta_0) > 0$ for antipolar (Chlamydomonas-like) microswimmers [24]. We consider only small asymmetry, $|\sin(\theta_0)| \approx |\theta_0| < 0.125$. Note that $|\sin(\theta_0)| \approx 0.5$ for sperms and Chlamydomonas [11], see also [12]. Furthermore, we apply a strong confinement with $L/l = 10$.

There are universal features in the behavior of an elongated microswimmer confined inside a channel. The swimmer performs a persistent random walk within the bulk region; when it encounters a wall, a torque, caused by steric interactions, leads to approximately parallel alignment with the wall; finally, the swimmer can escape from the boundary when its orientation, as a result of rotational diffusion, points slightly away from the boundary [4, 5]. Generally, swimmers are increasingly localized near the wall with increasing activity, as can be seen from the density profile $\rho(z)$ in Fig. 2(b). Shape asymmetry changes the behavior dramatically. Polar swimmers are much more strongly adsorbed as their antipolar counterpart, see Fig. 2(b). Moreover, polar particles point persistently toward the wall at an angle prescribed by the body shape, see high probability density at $(e_z,z) = (\sin(\theta_0),a/2)$ in Fig. 2(a) and compare to the probability density function $P(e_z,z)$ of an antipolar swimmer in Fig. 2(c). A high probability density near the boundary is tantamount to a large wall retention time. As can be seen in Fig. 3 and will be discussed in more detail below, the retention time of the particles indeed increases very rapidly with increasing activity and shape polarity.

In order to understand the giant wall accumulation of polar microswimmers, and in particular the huge trapping times, we examine Eqs. (1) and (2) with the focus on the two relevant variables, the coordinate along the surface normal $z$ and the orientation angle $\theta$, see Fig. 1, which implies
\[
\dot{z} = V\sin(\theta) + F_w/\gamma + \eta,
\]
\[
\dot{\theta} = -D_r \tan(\theta) + T_w/\gamma_r + \xi.
\]

The first term on the RHS of Eq. (4) is peculiar for rotational diffusion in 3D [14, 25] and can be neglected for $Pe \gg 1$. The noise obeys $\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$ with $D = k_BT/\gamma = (D_\parallel + 2D_\perp)/3$ and $\langle \xi(t)\xi(t') \rangle = 2D\delta(t-t')$. We linearize Eqs. (3) and (4) around the stable point $(z^*,\theta^*) = (a/2,\theta_0)$ of a fully absorbed particle, and define small perturbation as $(\delta z,\delta \theta) = (z-z^*,\theta-\theta^*)$. The equations of motion then reduce to an Ornstein-Uhlenbeck process,
\[
\frac{d}{dt} \begin{pmatrix} \delta z \\ \delta \theta \end{pmatrix} \approx \begin{pmatrix} \kappa V\theta_0 \\ 0 \end{pmatrix} \begin{pmatrix} V \\ \kappa^2V\theta_0 \end{pmatrix} \begin{pmatrix} \delta z \\ \delta \theta \end{pmatrix} + \begin{pmatrix} \eta \\ \xi \end{pmatrix},
\]
where we assume small $\theta_0$. Our aim is to estimate the mean escape time $\tau_e$, i.e., the mean time to reach an orientation parallel to the wall, $(z,\theta) = (a,0)$, from the stable position $(z,\theta) = (z^*,\theta^*)$ by rotational diffusion. In

![Fig. 2](color online) (a,c) Logarithmically color-coded plots of the probability density function (PDF) $P(e_z,z)$ at moderate activity $Pe = 8$. (a) $P(e_z,z)$ for a polar ($\theta_0 < 0$) and (c) an antipolar swimmer ($\theta_0 > 0$). Deterministic trajectories are indicated by solid lines. A polar swimmer is highly localised at $(e_z,z) = (\sin(\theta_0),a/2)$. (b) The corresponding orientation-averaged PDF $P(z)$ for $(\theta_0 = 0.1, Pe = 78)$. (d) PDF of the orientation $P(e_z,z \approx \delta)$ at the threshold of steric interactions $(\delta = l/2 + a)$, see dashed line in (a,c). Swimmers leave the wall region increasingly parallel with increasing $Pe$. 

![Fig. 3](color online) Logarithmically color-coded plots of the probability density function (PDF) $P(e_z,z)$ at moderate activity $Pe = 8$. (a) $P(e_z,z)$ for a polar ($\theta_0 < 0$) and (c) an antipolar swimmer ($\theta_0 > 0$). Deterministic trajectories are indicated by solid lines. A polar swimmer is highly localised at $(e_z,z) = (\sin(\theta_0),a/2)$. (b) The corresponding orientation-averaged PDF $P(z)$ for $(\theta_0 = 0.1, Pe = 78)$. (d) PDF of the orientation $P(e_z,z \approx \delta)$ at the threshold of steric interactions $(\delta = l/2 + a)$, see dashed line in (a,c). Swimmers leave the wall region increasingly parallel with increasing $Pe$. 

![Fig. 4](color online) Logarithmically color-coded plots of the probability density function (PDF) $P(e_z,z)$ at moderate activity $Pe = 8$. (a) $P(e_z,z)$ for a polar ($\theta_0 < 0$) and (c) an antipolar swimmer ($\theta_0 > 0$). Deterministic trajectories are indicated by solid lines. A polar swimmer is highly localised at $(e_z,z) = (\sin(\theta_0),a/2)$. (b) The corresponding orientation-averaged PDF $P(z)$ for $(\theta_0 = 0.1, Pe = 78)$. (d) PDF of the orientation $P(e_z,z \approx \delta)$ at the threshold of steric interactions $(\delta = l/2 + a)$, see dashed line in (a,c). Swimmers leave the wall region increasingly parallel with increasing $Pe$.
order to do so, we reduce the complexity of the problem further by neglecting the motion normal to the surface,
\[ \delta \theta = -\frac{dU}{d\theta} + \xi, \quad U = \frac{k}{2} \delta \theta^2. \tag{6} \]

Here, \( U \) is an effective harmonic potential for the orientation angle with spring constant \( k = -\kappa \gamma V \theta_0 / (4 \pi r). \)

The escape problem, Eq. (6), is related to a first passage problem. An exact expression of the mean first-passage time from any point along any potential to any other point exists \[26\]; however, due to the complexity of this expression, an extraction of the leading contributions seems unfeasible. A low-noise approximation is the Kramers rate theory of crossing a smooth potential barrier \[14, 26\]; here, we use a heuristic expression for the mean escape time over a barrier \( \Delta U = U(\delta \theta_c) = U(-\theta_0) \), which captures the low- and the high-noise limits \[3\],
\[ \tau_c = \frac{\delta \theta^2}{D_r} \exp \left( \frac{\Delta U}{D_r} \right) \right) \theta_0^2 \frac{\exp \left( \frac{\kappa l^2}{8D_r} V \theta_0 \right)}{\theta^3}. \tag{7} \]

Note that \( \theta_0 < 0 (\theta_0 > 0) \) for polar (antipolar) particles.

In the simulations, we mean the trapping time \( \tau_w \) as the time during which the swimmer remains within the wall region (range of steric interactions: \( z \in [0, \delta] \) or \( z \in [L - \delta, L] \) with \( \delta = l/2 + a \)). In case of polar swimmers, this trapping time is an estimate of \( \tau_c \). As can be seen in Fig. 3, we do indeed observe exponential dependencies of \( \tau_w \) in the low-noise regime, with \( \log (\tau_w) \propto \theta_0^3 \) in Fig. 3(a,b) and \( \log (\tau_w) \propto V \) in Fig. 3(c). The dependence of \( \tau_w \) on \( V \) is nicely consistent with Eq. (7); however, we observe \( \log (\tau_w) \propto \theta_0^3 \) instead of \( \log (\tau_c) \propto \theta_0^3 \), as predicted by Eq. (7). Considering the various approximations in the derivation of Eq. (7), like the harmonic form of \( U(\delta \theta) \) and the dimension reduction, it is not surprising that we do not obtain a perfect agreement. In particular, the parabolic description of \( U \) breaks down with increasing \( \delta \theta \); moreover, \( U \) is a function of \( \delta z \) and should soften with increasing \( \delta z \).

In case of apolar and antipolar swimmers, which do not point persistently toward the wall, the above treatment does not apply. Instead, \( \tau_w \) can be deduced from an analogy to a semi-flexible polymer adsorbed on a wall \[4, 5\], which predicts a scaling behavior \( \tau_w \propto V^{-2/3} \), see Fig. 3(c). This process contributes also to \( \tau_w \) of polar particles, but it becomes negligible as compared to the escape time over the effective potential barrier \( \Delta U \) for large polarity and \( Pe \gg 1 \).

The mean time \( \tau_b \), a swimmer remains within the bulk region (outside the range of steric interactions) is independent of \( \theta_0 \). As can be seen from Fig. 2(d), particles leave the wall region increasingly parallel with increasing \( Pe \). In agreement with the semi-flexible polymer analogy \[4\], we observe \( \langle \theta \rangle \propto V^{-1/3} \) at \( z \approx \delta \) in the ballistic regime. Thus, with \( \tau_b \propto L / (V \sin (\theta)) \) we obtain \( \tau_b \propto L / V^{2/3} \) consistently with simulations, see Fig. 3(d).

With this knowledge, it is easy to interpret a global measure of the density distribution, the surface excess (or adsorption) \( \Gamma = \int_0^L \left[ \rho(z) - \rho_b \right] dz \), where \( \rho_b \) is the bulk density. For a passive hard dumbbell, \( \Gamma = -\frac{\delta}{L - \delta} < 0 \), while for fully absorbed particles it is \( \Gamma = 1 \). A rough estimate of \( \Gamma \) is
\[ \Gamma \approx 2 \int_0^\delta \rho(z) dz - 2 \rho_b \delta \approx \frac{2 \tau_w - \tau_b \delta/(L - 2 \delta)}{2 \tau_w + \tau_b}. \tag{8} \]

Using the scaling of \( \tau_w \) and \( \tau_b \), see Fig. 3, we obtain low- and high-\( Pe \) limits, which are consistent with the simulation results, as indicated in Fig. 4(a).

The problem of a microswimmer with shape asymmetry moving near a planar wall bears a strong resemblance with a swimmer moving near a curved wall, see Fig. 5. Let us consider first a apolar swimmer in spherical confinement, see Fig. 5(a). In this case, as in the case of a polar microswimmer at a planar wall, the velocity vector in the stable conformation forms an angle with the tangent plane to the wall at the front bead. Thus, in both cases, the microswimmer points toward the wall and thus should have very long retention times. Secondly, the force of a polar microswimmer toward the wall can be partially or fully compensated by a negative curvature of the wall,
FIG. 4. (color online) (a) Adsorption $\Gamma$ versus activity $Pe$ for antipolar ($\theta_0 > 0$), apolar ($\theta_0 = 0$) and polar swimmer ($\theta_0 < 0$). Asymptotic estimates of $\Gamma$ are indicated by dashed lines. Note that polar swimmers are completely absorbed ($\Gamma = 1$) above a critical $Pe$, by contrast, apolar and antipolar swimmers are always partially absorbed. (b) $\Gamma$ as function of the asymmetry $\theta_0$ at various $Pe$.

FIG. 5. (color online) (a) An apolar swimmer confined within a spherical cavity of radius $R$ is equivalent to a polar swimmer close to a flat wall provided that the angle $\theta_0 \approx -l/(2R)$, between the propulsion force of the apolar swimmer and the tangent plane of the cavity at the front bead, equals the asymmetry $\theta_0 \approx (a_1 - a_2)/l$ of the polar particle. (b) A polar particle near a convex boundary behaves like an apolar swimmer close to a flat wall if $(a_1 - a_2)/l \approx -l/(2R)$.

i.e., for a microswimmer moving at the outer surface of a sphere, see Fig. 5(b). In the case of a full compensation, we predict the same accumulation behavior as for an apolar particle at a planar wall. Note that an apolar microswimmer would strongly scatter at negatively curved wall. Thus, shape polarity provides the possibility for microswimmers to move along curved surfaces!

We have tested our predictions for swimming near curved surfaces by simulating an apolar microswimmer inside a spherical confinement of radius $R$. The results for the wall retention times $\tau_w(Pe)$ and $\tau_w(\theta_0 \approx -l/(2R))$ [12] are in excellent agreement with the corresponding dependencies in Fig. 3(a,c). We have also verified the equivalence of a symmetric rod near a planar wall to a polar swimmer near a convex boundary provided that $(a_1 - a_2)/l \approx -l/(2R)$, see [12].

Hence, it is obvious to define a generalized asymmetry, considering shape asymmetry and wall curvature at once, as $\Theta_0 \equiv \theta_0^{shape} + g_0^{wall} = (a_1 - a_2)/l + kl/(2R)$ for $R \gg l \gg |a_1 - a_2|$, where $k = +1$ for convex and $k = -1$ for concave boundaries. This allows a unified description of asymmetric microswimmers near curved walls, where $\Theta_0 < 0$ ($\Theta_0 > 0$) implies an exponential growth (algebraic decay) of $\tau_w$ with $V$.

Finally, we want to briefly discuss the the wall pressure in active systems. There are several attempts to construct an equation of state for active fluids [27–29]. However, this idea has been questioned, because the pressure $p$, measured as the force exerted on the boundary per wall area, should strongly depend on the details of the swimmer-wall interaction [30], in contrast to thermal equilibrium. Our results support the latter claim. We observe that, in contrast to active Brownian spheres where $p \propto V$ in the strong confinement limit ($Pe \gg L/l$) [27], $p \propto V^{1.35}$ for polar swimmers, and $p \propto V^{0.42}$ for symmetric rods and antipolar particles, see Fig. 6. The difference between a spherical and a rod-like particle is that the latter exert a significant force only during the arrival at the wall, and align immediately parallel with the boundary due to the steric torque $T_w(e_z, z)$.

In summary, we have shown that a small shape polarity of microswimmers leads to extremely long wall-trapping times. The exponential dependence of $\tau_w$ on $V$ and $\theta_0$ is responsible for a nearly complete adsorption of polar particles, in contrast to symmetric or antipolar particles. The pressure $p$ in active system is sensitive to the details of the swimmer-wall interaction [30], in particular the variation of the asymmetry from antipolar to polar change the grow of $p$ with $V$ from sublinear to superlinear. Furthermore, we have shown that wall curvature can compensate the effect of shape asymmetry, i.e., asymmetry and curvature are two sides of the same coin. Thus, the combination of both effects can be used in order to design artificial microswimmers or microfluidic devices for particular tasks. For example, microswimmers could be designed which move along surfaces within a porous medium [19, 31], while corrugated microfluidic channels can be constructed to reduce wall accumulation [7, 21].
Wherever appropriate, we choose realistic parameters. In reality, however, cells usually do not exhibit such high face curvature, which is claimed in the main text. Most theoretical studies of simple model swimmers, both in bulk and confinement, have considered cells with a symmetric body shape, in particular rods and spheres. In reality, however, cells usually do not exhibit such high symmetry, as demonstrated by the stroke-averaged shape of sperm and Chlamydomonas, see Fig. 7, which rather resembles a forward or a backward swimming cone, respectively. We have performed various simulations in order to test and verify the equivalence of shape asymmetry and surface curvature, which is claimed in the main text.

First, we analyse the behavior of an apolar microswimmer ($\theta_0^{\text{shape}} = 0$) close to a surface with a curvature ranging from that of a convex to a concave body. The wall retention times $\tau_w$ as a function of the wall asymmetry $\theta_w = k l/(2 R)$ are shown in Fig. 8(a,b). The results bear a close resemblance to those in Fig. 9(a,b).

**SUPPLEMENTARY MATERIALS**

Most theoretical studies of simple model swimmers, both in bulk and confinement, have considered cells with a symmetric body shape, in particular rods and spheres. In reality, however, cells usually do not exhibit such high symmetry, as demonstrated by the stroke-averaged shape of sperm and Chlamydomonas, see Fig. 7, which rather resembles a forward or a backward swimming cone, respectively.

![Image](image.jpg)
FIG. 8. (color online) Influence of the boundary curvature on the behaviour of an apolar microswimmer ($\theta_0^{shape} = 0$). $\theta_0^{wall} = -l/(2R) < 0$ corresponds to a motion within a spherical cavity of radius R and $\theta_0^{wall} = l/(2R) > 0$ means swimming close to the outer surface of a sphere with radius R. (a) $\tau_w$ versus $\theta_0^{wall}$ and (b) $\tau_w$ versus $Pe$. Note that $\tau_w \propto V^{-1}$ for $\theta_0^{wall} > 0$ in contrast to $\tau_w \propto V^{-0.7}$ for $\theta_0^{wall} = 0$ (flat wall).

FIG. 9. (color online) Asymmetric swimmer near a flat wall ($\theta_0^{wall} = 0$). Same figure as Fig. 3(a,b) of the main text, reproduced here for easier comparison. Note that $\theta_0^{shape} < 0$ ($\theta_0^{shape} > 0$) for polar (antipolar) particles. (a) $\tau_w$ versus $\theta_0^{shape}$ and (b) $\tau_w$ versus $Pe$. For polar swimmers $\tau_w$ grows exponentially with $V$, while for apolar and antipolar swimmers $\tau_w \propto V^{-0.7}$.

FIG. 10. (color online) A polar swimmer near a convex body (a sphere of radius R). We fix the shape polarity $\theta_0^{shape} = -0.09$ and vary $\theta_0^{wall} = l/(2R)$ by changing $R$. In the following we use the generalized asymmetry $\Theta_0 \equiv \theta_0^{shape} + \theta_0^{wall}$. (a) $\tau_w$ versus $\Theta_0$ and (b) $\tau_w$ versus $Pe$. Note that for $\Theta_0 \approx 0$ the negative curvature of the wall compensates the shape polarity and a polar microswimmer behaves like an apolar particle near a plane wall.

and Fig. 9(a,b) is striking. Hence, if shape and wall polarity cancel, i.e., $\Theta_0 \approx 0$, a polar microswimmer close to a convex boundary behaves similar to an apolar swimmer near a flat wall.