Substrate elasticity tunes the dynamics of polyvalent rolling motors

Supplementary material

December 4, 2020

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Single trajectory analysis

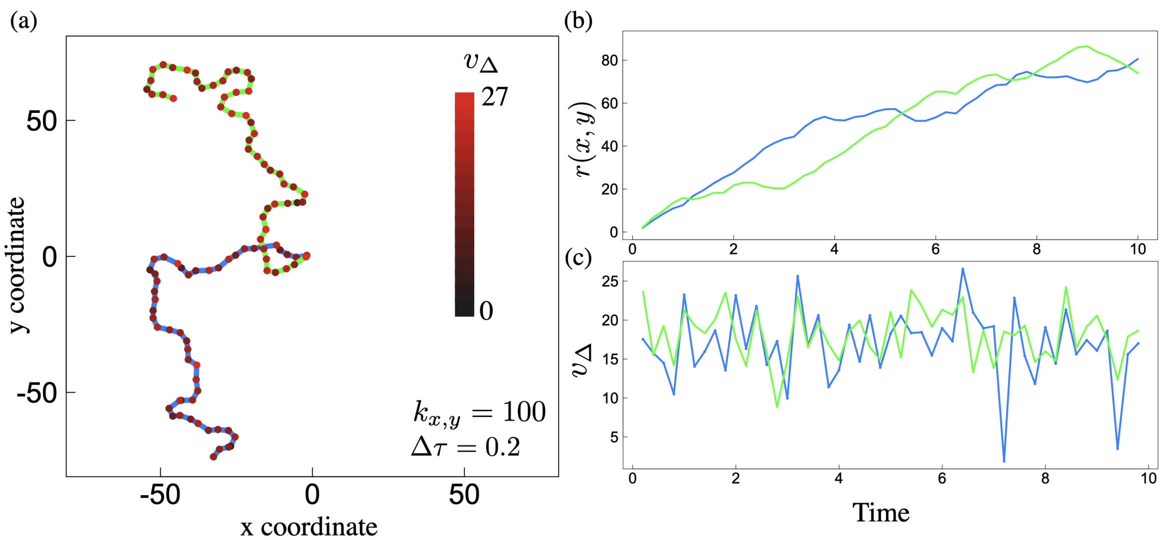

Figure S1: a) Two trajectories from the $k_{x,y} = 100$ ensemble were randomly chosen for analysis. Trajectory positions are denoted by green and blue lines, where the points are coloured according to their instantaneous speed at that position in time. The average speed throughout the trajectory is 18.1 and 16.8 with α_{TA} of 1.68 and 1.49 for the green and blue trajectories, respectively. (b) $r(x, y)$ as a function of time. (c) v_Δ as a function of time computed over a $\Delta\tau$ interval of 0.2, where $v_\Delta(\tau) = \frac{\sqrt{(x(\tau+\Delta\tau)-x(\tau))^2+y(\tau+\Delta\tau)-y(\tau))^2}}{\Delta\tau}$.

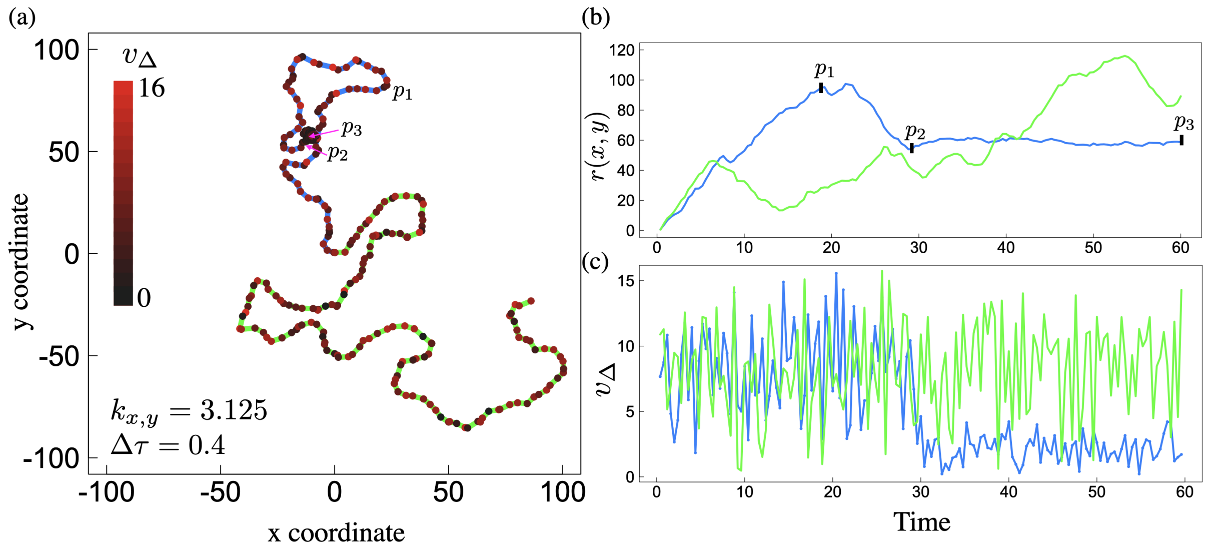

Figure S2: a) Two trajectories from the $k_{x,y} = 3.125$ ensemble were chosen: the blue trajectory is an example of a bead traversing into an area surrounded by product sites, thereby persisting in a long product-entrapped state, while the green trajectory is an example of a bead that avoids becoming 'trapped' by surrounding product sites, thereby persisting in a substrate-driven state. α_{TA} are 1.68 and 1.51 for the green and blue trajectories, respectively. (b) $r(x, y)$ as a function of time. p_1 is an example where the relative position $r(x, y)$ appears to be constant however the local speed is non-zero; here the bead may appear to be trapped if velocity is computed relatively, versus a local speed as shown in (c). p_2 is the point at which the bead actually becomes trapped by product sites. p_3 is the end-point of the trajectory. (c) v_Δ as a function of time computed over a $\Delta\tau$ interval of 0.4. For the blue trajectory the average speed from $t = 0$ to p_2 is 8.3, and the average speed from p_2 to p_3 is 2.3. The average speed of the green trajectory is 8.2.

First passage time for $N_B = 0$ for all $k_{x,y}$ ensembles

Because detachment can strongly bias dynamical measures inferred from MSD analysis we wanted to determine whether detachment was responsible for the ensemble 'acceleration' inferred from superballistic values of $\alpha_{\rm EA}$ in Fig. 2b. Thus, in Fig. S3 we plot the average time to the first observed detachment event (the first passage time, FPT, to $N_{\rm B} = 0$) as a function of $k_{x,y}$. We find that the FPT increases with an increase in $k_{x,y}$, suggesting that stiffer substrates support more processive trajectories. Note that, because the plotted FPT is an average FPT only for those trajectories exhibiting detachment ($N_{\rm B}$=0), it underestimates the true mean FPT because many trajectories do not detach on the timescale of our simulations (Fig. 6).

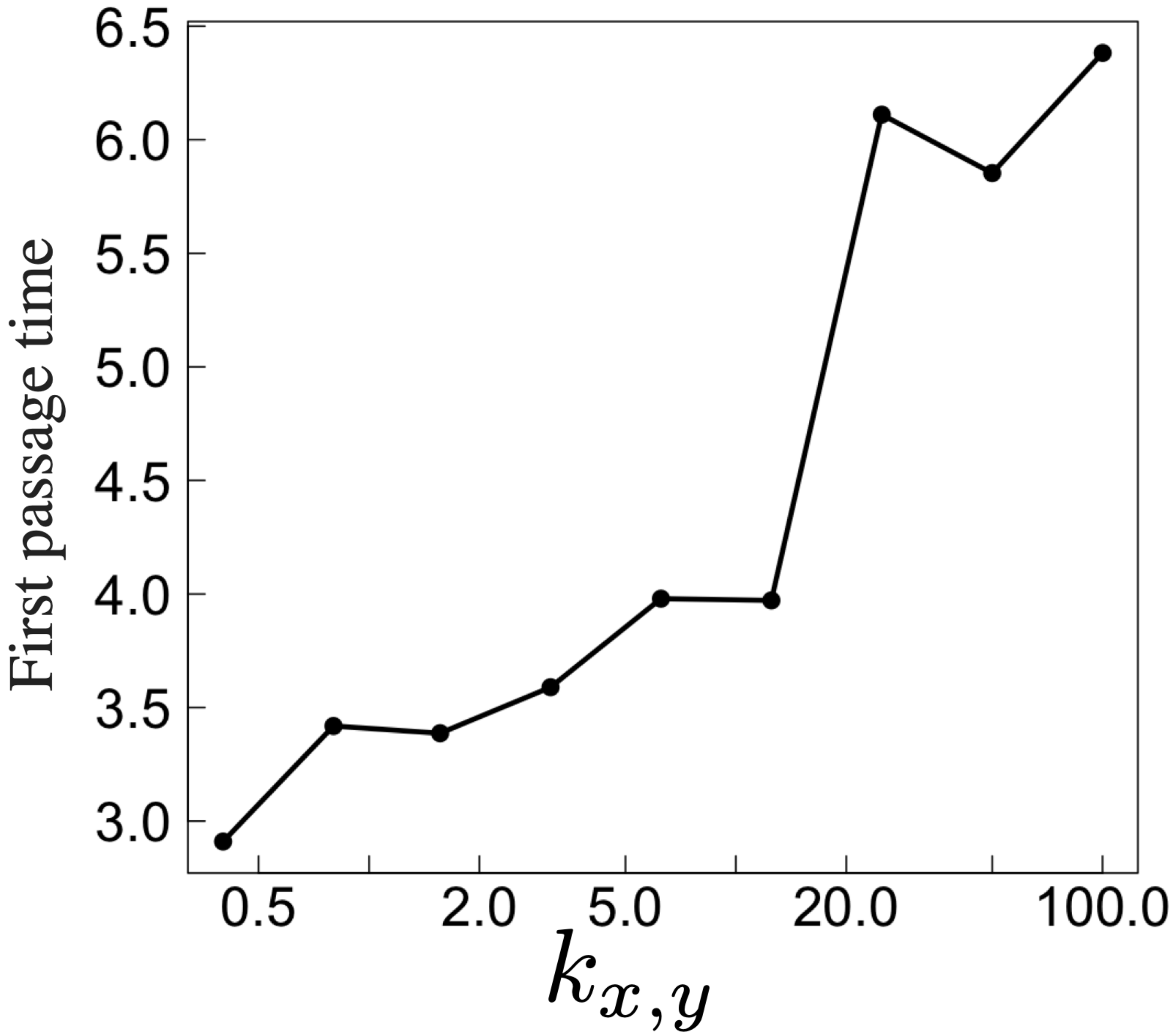

Figure S3: Average first passage time to detachment (defined here as $N_{\rm B} = 0$) as a function of $k_{x,y}$.

MSD_{TA} calculations

The trajectory-averaged MSD displays a similar trend as a function of time lag for all elasticities (Fig. 2d). The scatter of calculated α values for different trajectories is shown in Figure S4a. In Figure S4b we plot the generalized diffusion coefficient as a function of bead index for each $k_{x,y}$ ensemble. We find that the diffusion coefficient is highly dependent on $k_{x,y}$, where for stiff substrates ($k_{x,y} = 100$) it maximizes at $A \approx 200$ before decreasing to $A \approx 50$ for soft substrates ($\mathrm{k_{x,y}} = 1.5625$).

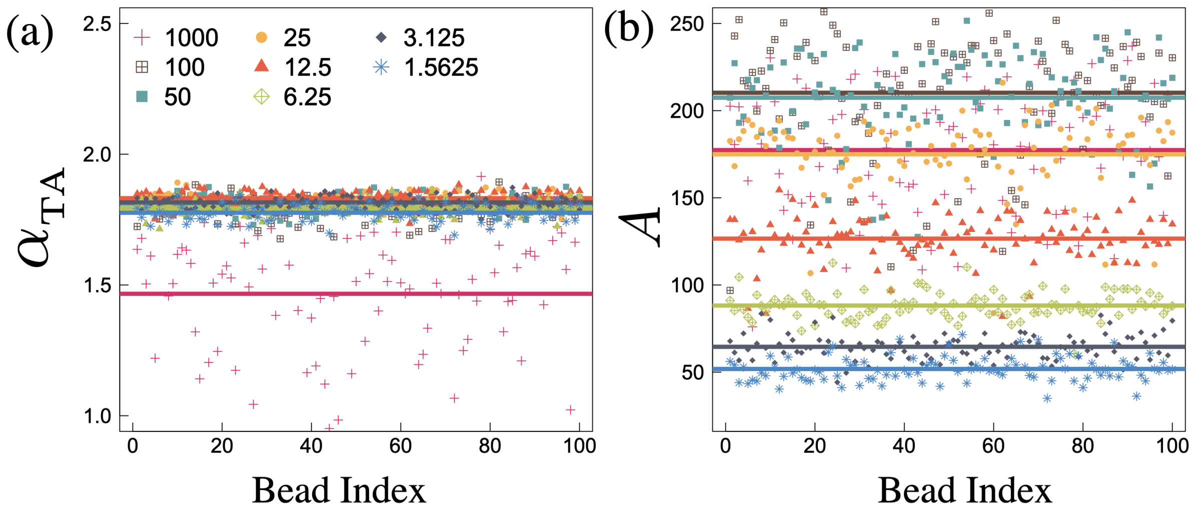

Figure S4: a) Scatter plot of α_{TA} for all 100 polyvalent spheres in each $k_{x,y}$ ensemble. b) Scatter plot of the generalized diffusion coefficient for all 100 polyvalent spheres in each $k_{x,y}$ ensemble.

Scatter plots of Δ_x versus Δ_{θ_y}

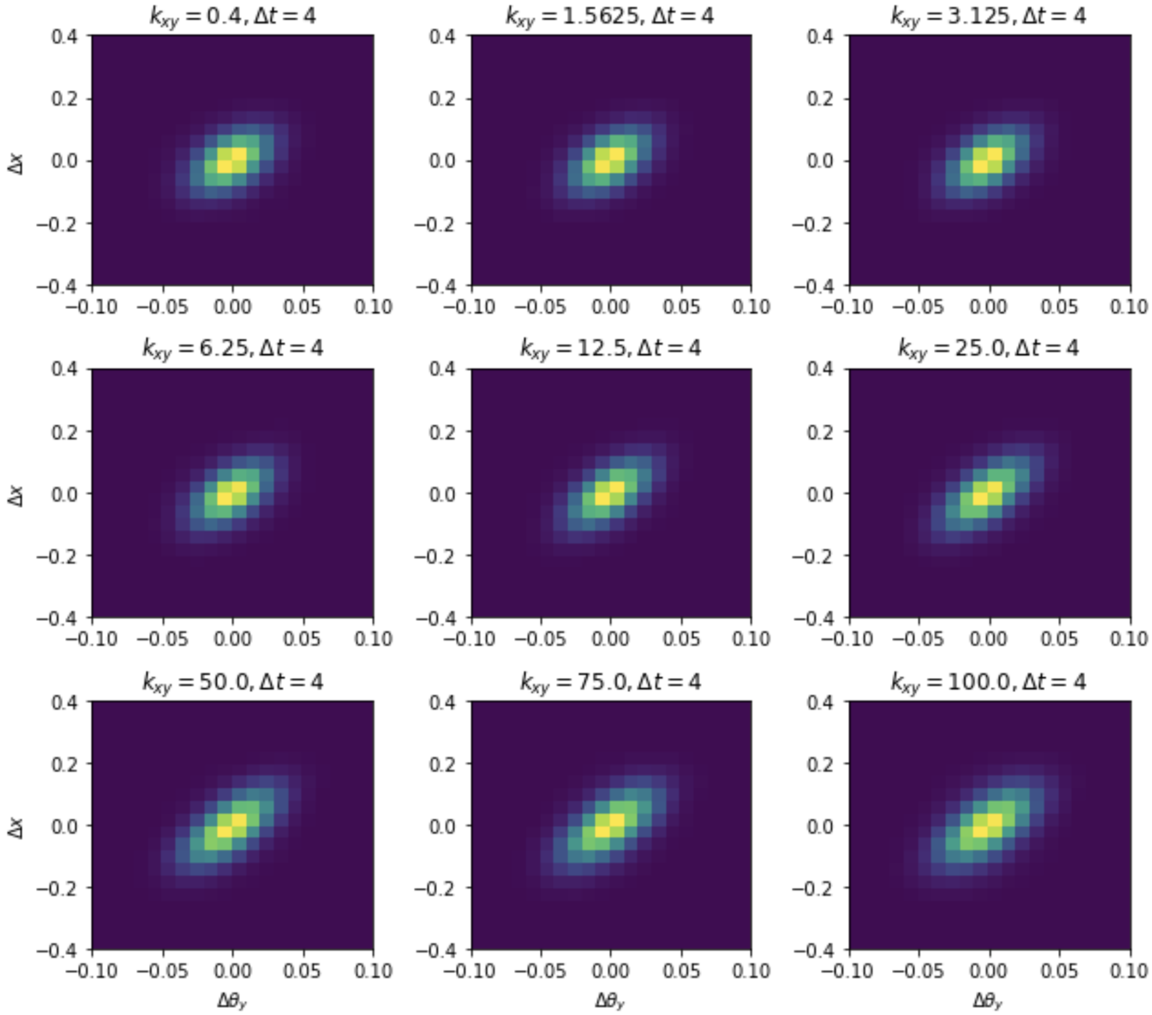

Figure S5: Scatter plots of translational versus angular displacements on substrates of different stiffness. Shown are Δx versus $\Delta\theta_y$ calculated for a time lag of $\Delta\tau = 4\tau_{int} = 0.004$. The correlation is low, but increases with increasing substrate stiffness, $k_{x,y}$.

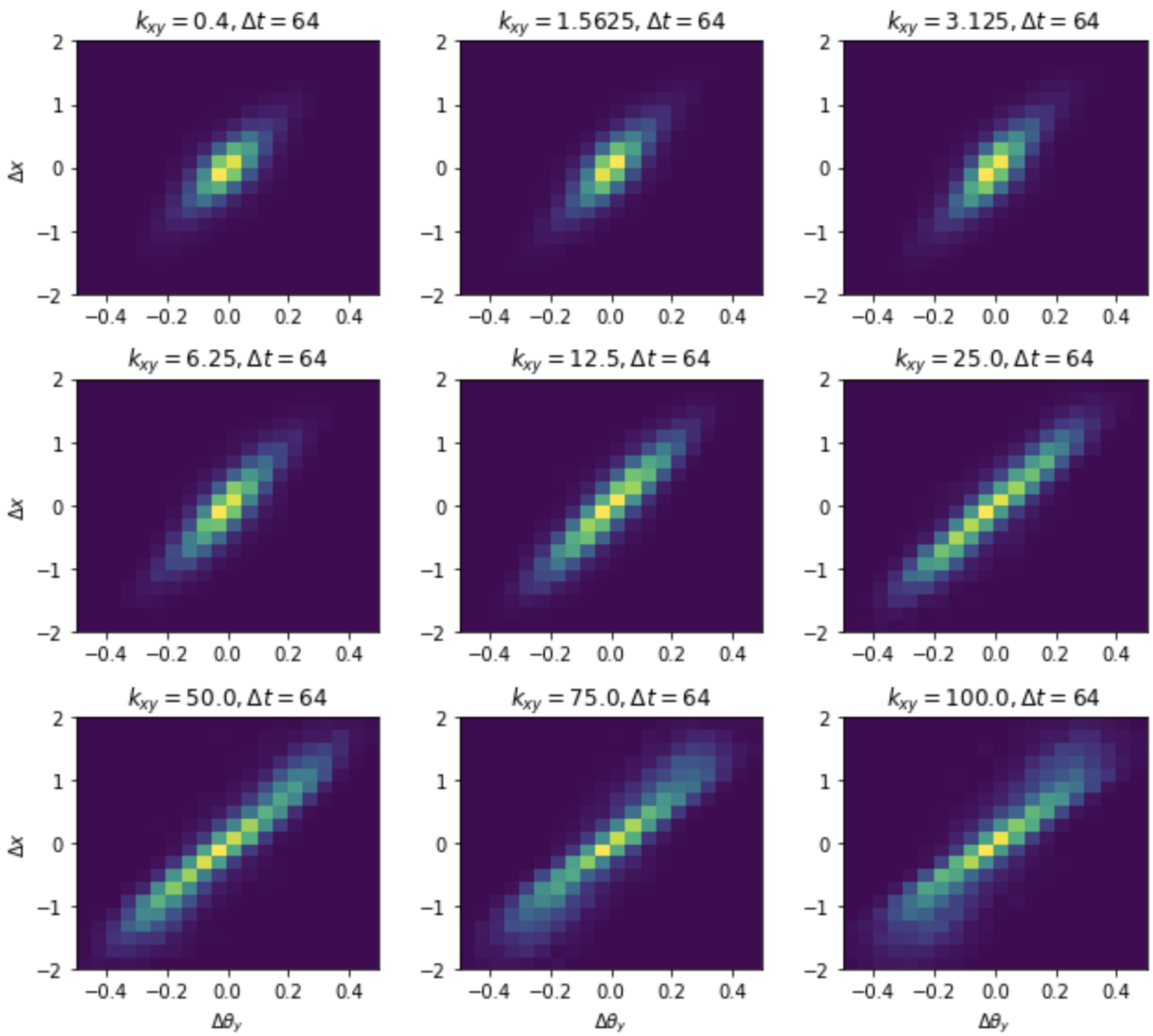

Figure S6: Scatter plots of translational versus angular displacements on substrates of different stiffness. Shown are Δx versus $\Delta\theta_y$ calculated at a time step of $\Delta\tau = 64\tau_{int} = 0.064$. The correlation is much stronger than in Fig.S5, and increases with increasing substrate stiffness, $k_{x,y}$. These plots were used to calculate the correlation coefficients shown in Fig. 4.

Processivity analysis with reduced substrate occupancy, p

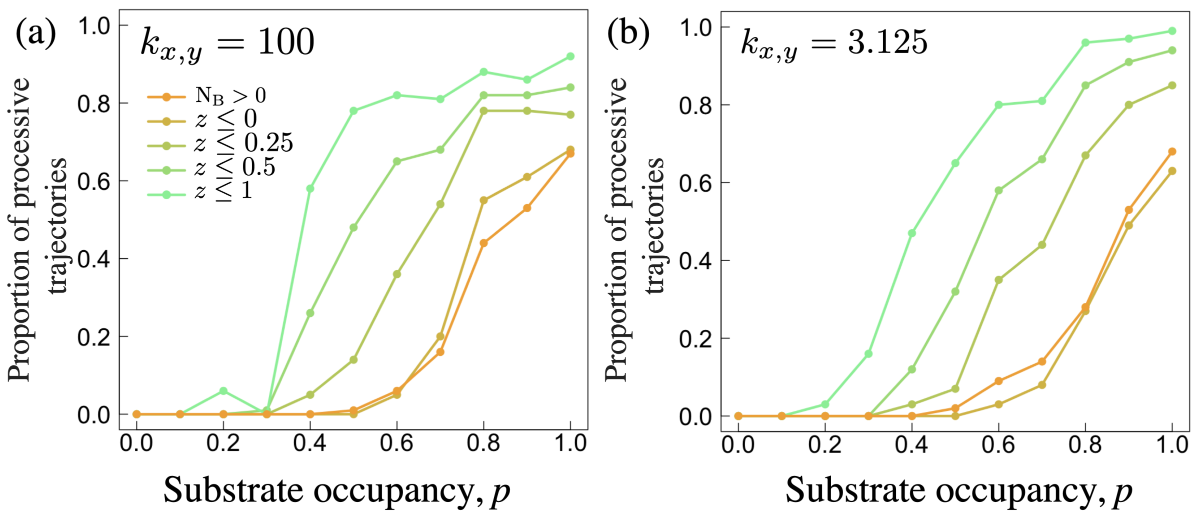

Figure S7: Procssivity analysis for soft $k_{x,y} = 3.125$ and rigid $k_{x,y} = 100$ substrates as a function of substrate occupancy, p. We find agreement between using number of bound substrate as well as a height cutoff of $z < 0$ as metrics for processivity. As the height cutoff is relaxed subtle differences of processivity between soft and rigid substrates emerge, where softer substrates tend to be more processive.

$\mathrm{MSD}_{\mathrm{EA}}$ calculations for various p on $\mathrm{k}_{\mathrm{x,y}} = 100$

To demonstrate the effects of substrate occupancy on polyvalent sphere kinetics we compute the $\mathrm{MSD}_{\mathrm{EA}}$ for all substrate occupancies explored on the stiff lattice (Fig. S8).

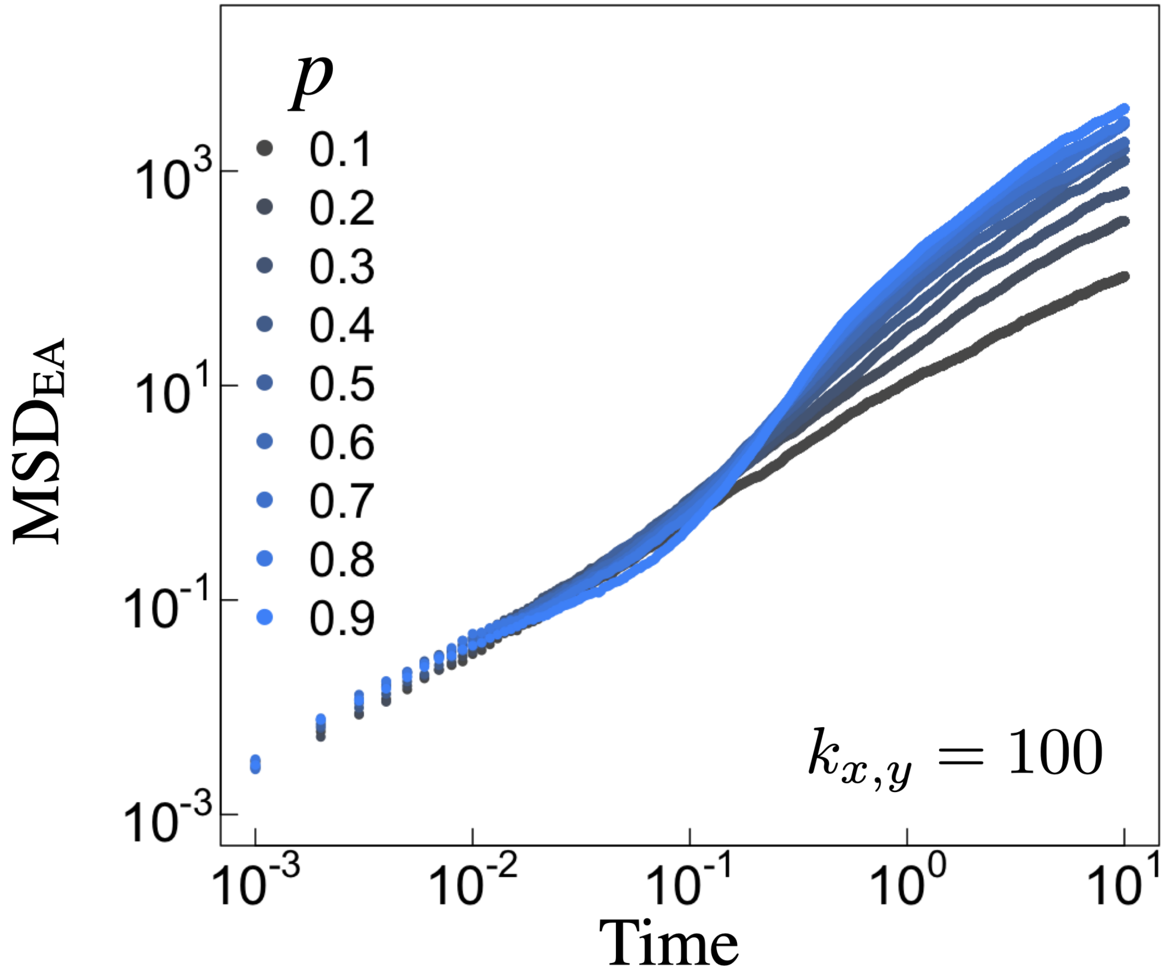

Figure S8: $\mathrm{MSD}_{\mathrm{EA}}$ analysis of stiff substrates ($k_{x,y} = 100$) with varying occupancy.

As the substrate occupancy decreases down to $p = 0.1$ the system becomes more conventionally diffusive, with the $\mathrm{MSD}_{\mathrm{EA}}$ at $p = 0.1$ resulting in α_{EA} close to the Brownian limit of 1.0.

Supplementary movies

Movie S1: Motion of a spherical BBR on a 2D surface of substrates with varying planar elasticity. The top panels show the time evolution of the motor on a substrate with elasticity, $k_x = k_y = k_z = 100$. The left panel shows the substrate cleavage and the right panel shows the rotation of the BBR where the frame of reference has been centred at the centre of mass of the motor. Possible detachment events have been shown. The bottom panels show the time evolution for elasticity, $k_x = k_y = 3.125$, $k_z = 100$ for the same frame rate as the top panels. Again, the left panel shows the substrate cleavage and the right panel shows motor rotation.