Supplementary Material: Conformational Behavior and Self-Assembly of Disjoint Semi-Flexible Ring Polymers Adsorbed on Solid Substrates

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Overlap Density

Since in the present article, we frequently refer to the overlap density, we provide in this supplementary a rationale and values of the overlap density, ρ^* in the case of uniform substrates. In the case of polymer chains, the overlap density in two dimensions is typically defined as $\rho^* \approx 1/R_g^2$, where R_g is the radius of gyration of the polymer in the dilute regime. However, since R_g is smaller than the real size of the molecule, we use a more accurate definition of the size of the ring polymer defined as the ensemble average of the maximum distance between monomers of a ring polymer and its center of mass in the dilute regime. This length scale, R_{max} is proportional to the radius of gyration of the polymer. The overlap density, defined as $\rho^* \approx 1/R_{max}^2$ is shown versus the bending rigidity of the polymers, κ, in Fig. S1. This figure shows that the overlap density decreases with increasing κ up to about $\kappa \approx 5k_BT$, which is inline with the fact that the degree of anisotropy of the polymers increases with κ (i.e., a decrease in Σ) for low values of κ as shown by Fig. 3. However, for $\kappa \gtrsim 5k_BT$, ρ^* weakly increases with κ, which is also inline with the decrease in the degree of anisotropy (or increases in Σ) for large values of κ as shown by Fig. 3.

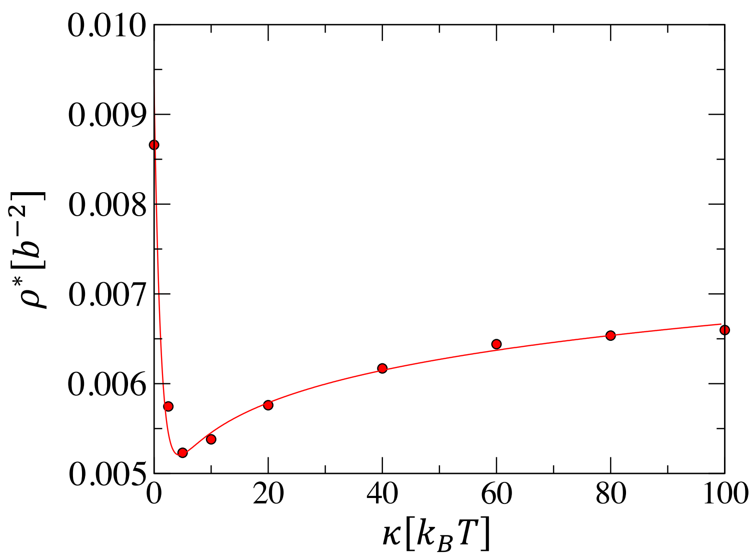

Figure S1: Solid circles correspond to the overlap density of the ring polymers versus their bending rigidity in the case of a uniform substrate. The solid line is a guide to the eye.

Curvature Distribution

Fig. S2 shows the distribution of the local curvature, $D(c)$ for the case of $\kappa = 100k_BT$ at different densities. Notice that the peak is at a finite value of c for densities lower than $0.01b^{-2}$. However, for densities higher that $0.01b^{-2}$, the peak shifts to $c \approx 0$, and a shoulder emergence at large positive values of c. The change in the shape of the distribution is correlated with the change of the morphology of the polymers from mainly obround to biconcave.

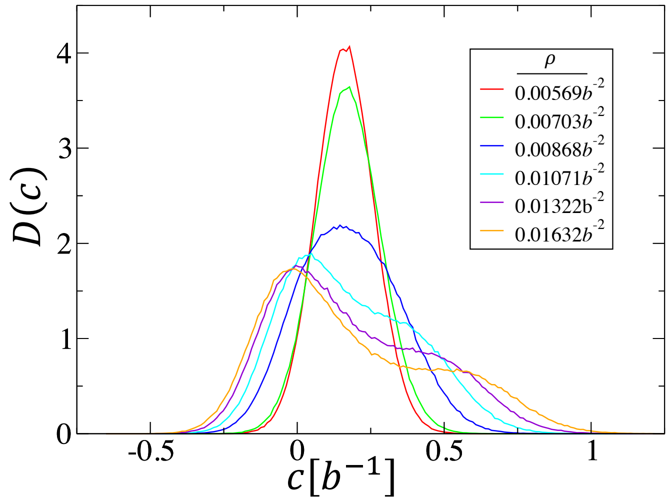

Figure S2: Normalized curvature distribution for the case of $\kappa = 100k_BT$. Data correspond to different densities shown in the legend. Notice the emergence of a shoulder at high curvatures for $\rho > 0.01b^{-2}$ and a shift of the main peak's position to the left as ρ is increased.

Positional and Nematic Correlations

Fig. S3 depicts the positional pair correlation, calculated using Eq. (13) of the main text, in the case of low bending rigidity ($\kappa = 5k_BT$) and high bending rigidity ($\kappa = 80k_BT$).

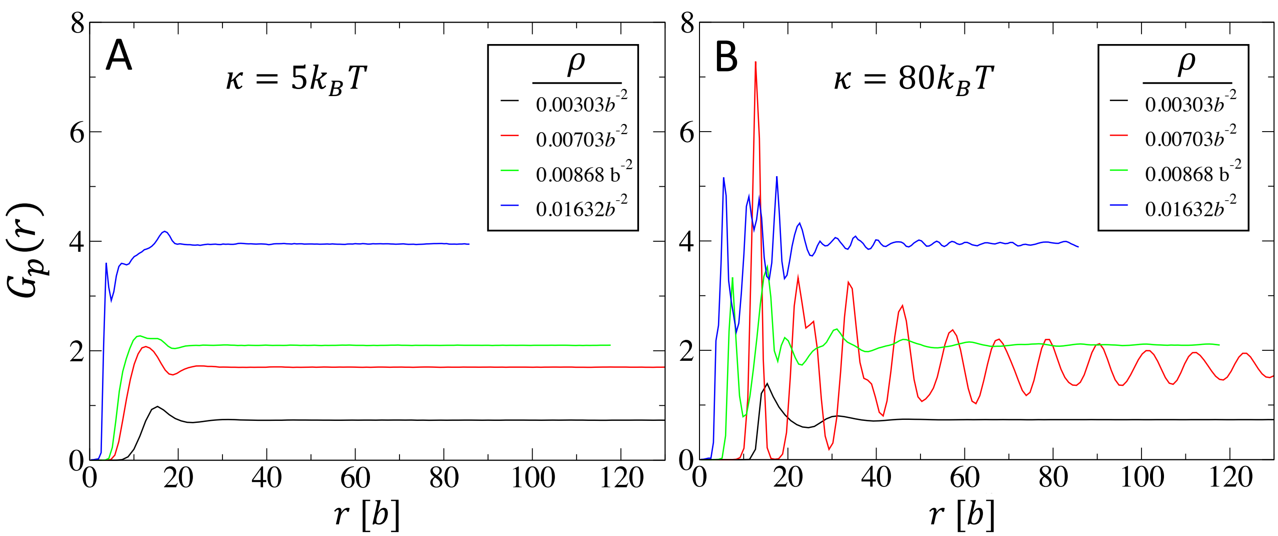

Figure S3: Positional correlation function $G_p(r)$ versus r for different values of the density. (A) and (B) corresponds to $\kappa = 5k_BT$ and $80k_BT$, respectively.

Fig. S4 depicts the orientational pair correlations in the case of low bending rigidity ($\kappa = 5k_BT$) and high bending rigidity ($\kappa = 80k_BT$). The orientational pair correlations is calculated using

$$G_n(r) = \left\langle \cos 2\left[\theta\left(\mathbf{R}_k\right) - \theta\left(\mathbf{R}_l\right)\right] \delta\left(\mathbf{r} - \mathbf{R}_{kl}\right) \right\rangle, \tag{1}$$

where $\mathbf{R}_k$ and $\mathbf{R}_l$ are the coordinates of the centers of mass of polymers k and l, and $\theta(\mathbf{R}_k)$ is the angle between the director of polymer k and an arbitrary fixed axis.

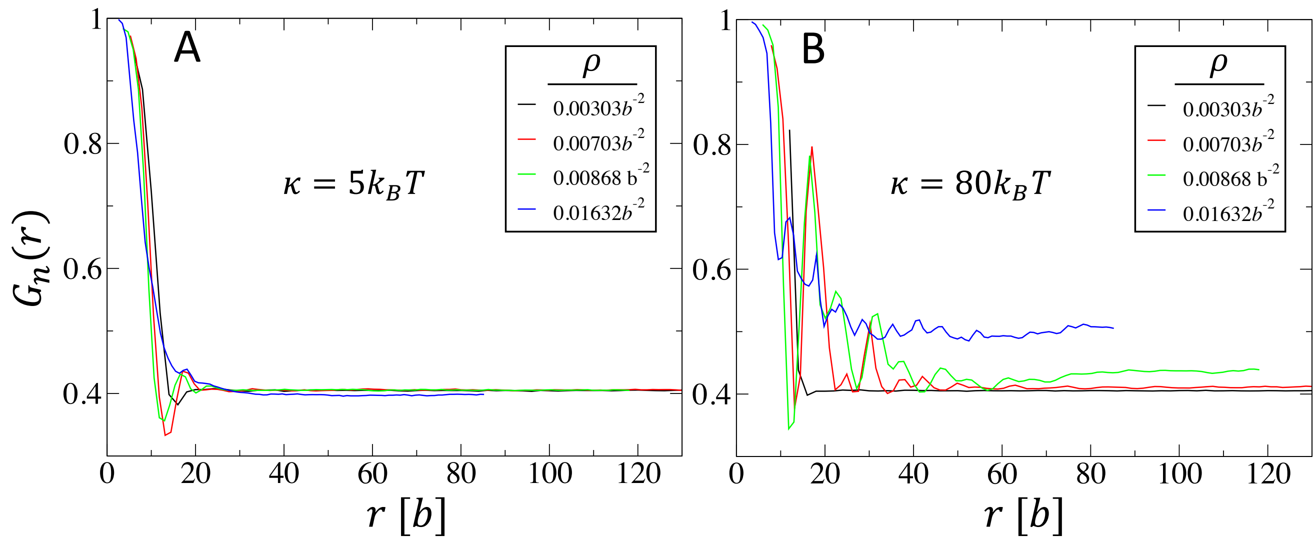

Figure S4: Nematic correlation function $G_n(r)$ versus r for different values of the density. (A) and (B) corresponds to $\kappa = 5k_BT$ and $80k_BT$, respectively.