Supporting Information for

Weak Shape Anisotropy Leads to a Non-monotonic Contribution to Crowding Impacting Protein Dynamics under Physiologically Relevant Conditions

Jin Suk Myung,*,† Felix Roosen-Runge,*,† Roland G. Winkler,‡ Gerhard Gompper,‡ Peter Schurtenberger,† and Anna Stradner*,†

†*Division of Physical Chemistry, Department of Chemistry, Lund University, SE-221 00 Lund, Sweden*

‡*Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany*

E-mail: jin_suk.myung@fkem1.lu.se; felix.roosen-runge@fkem1.lu.se; anna.stradner@fkem1.lu.se

Deformation of ellipsoids

The deformation of ellipsoids is calculated by the difference between the measured radius and the initial radius of ellipsoids. (Figure S1).

Intermediate scattering function

The short-time collective diffusion coefficient $D_s(q)$ (cf. Figure 2) is extracted from a single exponential fit to the short-time part of the intermediate scattering function

$$S(q,t) \approx S(q,0)e^{-q^2 D_s(q)t} \tag{S1}$$

where the intermediate scattering function (Figure S2A) is calculated by

$$S(q,t) = \left\langle \frac{1}{N} \sum_{j,k}^{N} e^{i\mathbf{q}\cdot(\mathbf{r_j(0)} - \mathbf{r_k(t)})} \right\rangle . \tag{S2}$$

Note that only the short-time part of $S(q,t)$ is used for the fit ($t \leq 0.2\tau$, where $\tau = {R_h}^2/D_0$ is the characteristic time of colloids).

Mean-square-displacement

The short-time self-diffusion coefficient D_s^s (cf. Figure 3) is calculated from the mean-square-displacement $\langle \Delta r^2 \rangle = 6D_s^s t$ of colloids (Figure S2B). Note that only the short-time linear part of the MSD is used for the fit ($t \leq 0.6\tau$).

Number of connected neighbors

The local environment of individual colloids is analyzed by the average number of connected neighbors N_{nbr} (i.e. belonging to the same cluster) within a cutoff radius $R_{cut} = 7R_h$ of attractive spheres and ellipsoids as a function of volume fraction (Figure S3), which is normalized by the number density, $N^*_{nbr} = N_{nbr}/[(N/L_s^3) \times (\frac{4}{3}\pi R_{cut}^3) - 1]$. Here, two colloids are considered as connected neighbors when their bead separation is smaller than the distance at the first minimum of the pair correlation function ($r \leq 1.4\sigma$), and the cutoff radius R_{cut} is set to eliminate the effect of the simulation box size in the analysis.

Orientational angle distribution

The orientational ordering of ellipsoids is analyzed by the distributions $P(\cos(\theta))$ of angles θ between neighboring ellipsoids (Figure S4). The orientation of an ellipsoid is defined by its semi-principal axis r_a, where the angle $\cos(\theta)$ of two ellipsoids varies from 0 for perpendicular orientation to 1 for parallel orientation.

Structure factor

The characteristic of the structure can be analyzed by the structure factor (cf. Figure 5)

$$S(q) = 1 + \frac{N}{V} \int_0^\infty 4\pi r^2 \left[g(r) - 1\right] \frac{\sin\left(qr\right)}{qr} dr \tag{S3}$$

where the the pair-correlation function

$$g(r) = \frac{V}{N^2} \left\langle \sum_i \sum_{j \neq i} \delta(\mathbf{r} - \mathbf{r}_{ij}) \right\rangle \tag{S4}$$

is the probability to find a pair of colloids a distance r apart.

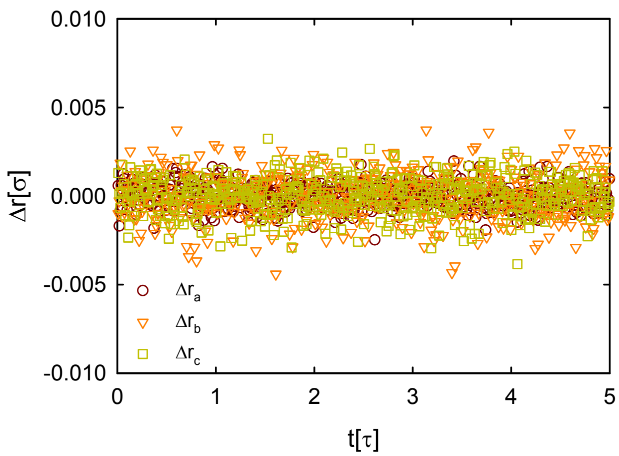

Figure S1: Deformation of ellipsoids.

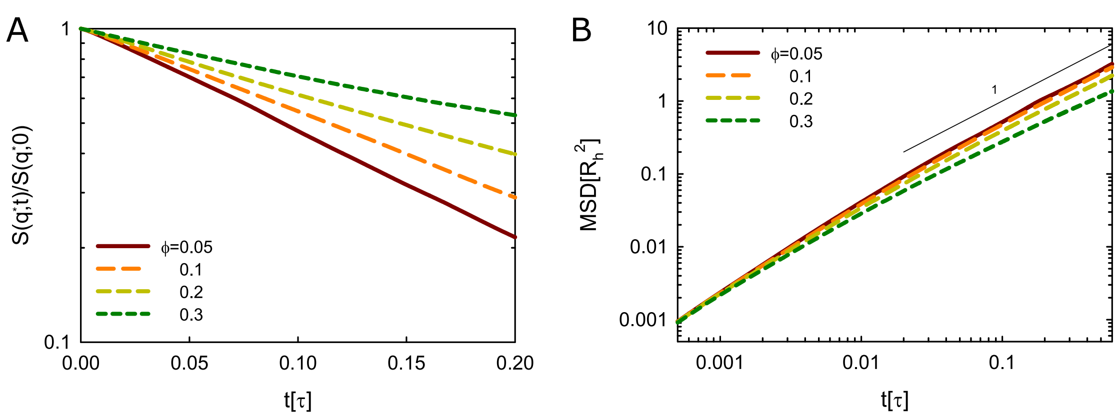

Figure S2: (A) Intermediate scattering function (ISF) for different volume fractions of hard ellipsoid. The ISF of $0.02\tau \leq t \leq 0.2\tau$ is used for the fit to obtain the short-time collective diffusion coefficient $D_s(q)$. (B) Mean-square- displacement (MSD) for different volume fractions of hard ellipsoid. The MSD of $0.02\tau \leq t \leq 0.6\tau$ is used for the fit to obtain the short-time self-diffusion coefficient D_s^s.

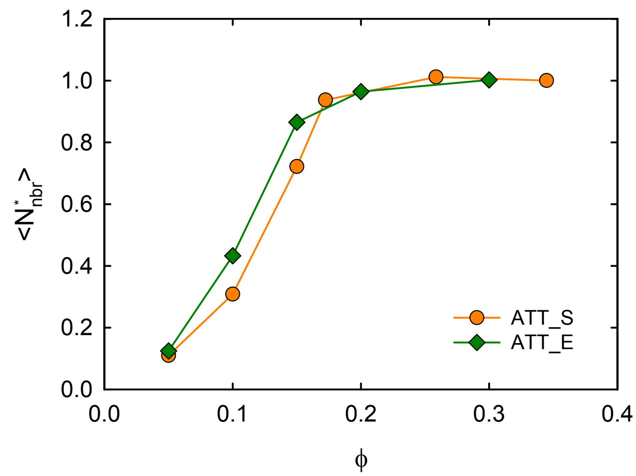

Figure S3: Normalized average number of connected neighbors N^*_{nbr} within a cutoff radius $R_{cut} = 7R_h$ of attractive spheres (ATT_S) and ellipsoids (ATT_E) as a function of volume fraction.

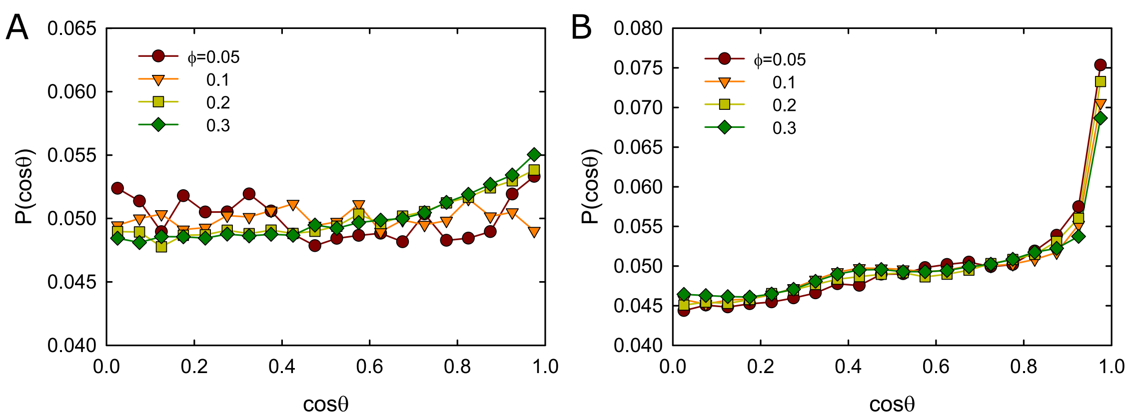

Figure S4: Distributions of angles θ between neighboring (A) hard and (B) attractive ellipsoids for different volume fractions.