

Electronic Supplementary Information for

The kinetic friction coefficient of neutral and charged polymer brushes

Florent Goujon ^a, Aziz Ghoufi ^b, Patrice Malfreyt ^{*a} and Dominic J. Tildesley ^a

^a Clermont Université, Université Blaise Pascal, Institut de Chimie de Clermont-Ferrand, ICCF, CNRS, UMR 6296, BP 10448, F-63000 Clermont-Ferrand, France. Fax: +33 473 40 53 28; Tel: +33 473407204; E-mail: Patrice.Malfreyt@univ-bpclermont.fr

^b Institut Physique de Rennes, UMR CNRS 6251, IPR, 263 Avenue Général Leclerc, F-35042 Rennes, France.

The calculation of the profiles of the shear forces was decomposed into several block averages for neutral polymer brushes at equilibrium and under shear for the smallest shear rate used here ($\dot{\gamma}_a = 0.0001$). With 7 block-averages, the average of p_{xz} at equilibrium is $(-2.2 \times 10^{-4} \pm 2.5 \times 10^{-4})$ and under shear $(-6.5 \times 10^{-4} \pm 1.7 \times 10^{-4})$. We only represent the profiles of 3 block averages for clarity in Fig. S1. As expected from the mechanical equilibrium, the average of p_{xz} over the different blocks is scattered around zero whereas the average value of the shear forces is negative at the smallest shear rate. Fig. S1 shows that there is an overlap between the profiles obtained at equilibrium and under shear establishing that the shear rate of 10^{-4} is the smallest value we can simulate with reasonable system size (20000 DPD particles) and simulation time (125 CPU hours for 3×10^6 time steps).

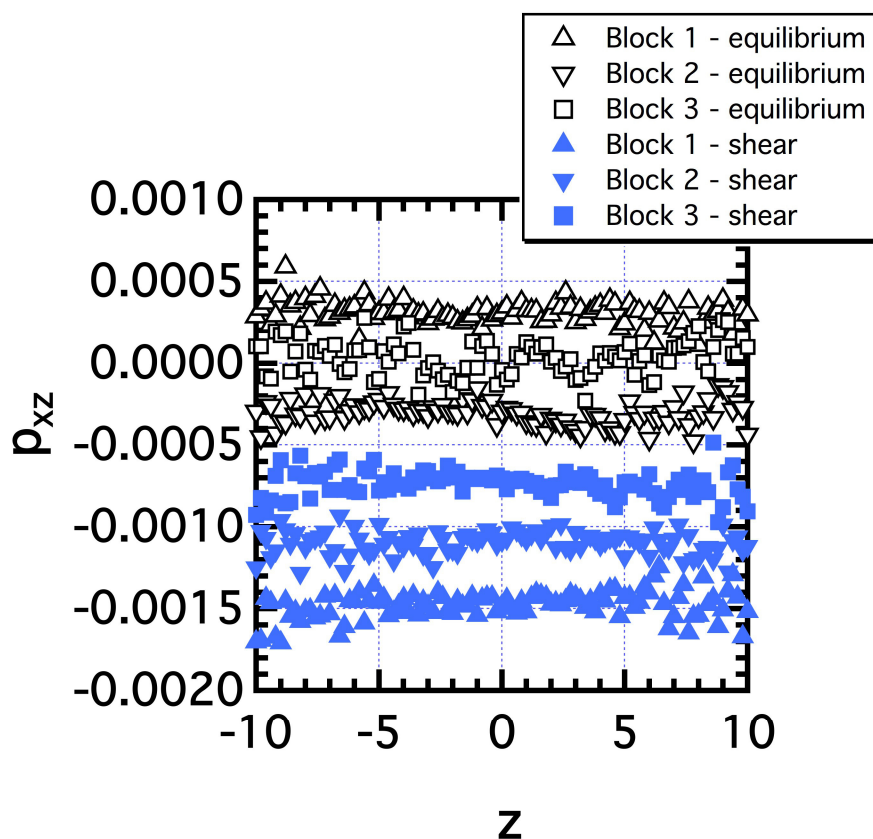


Fig S1: Profiles of the shear forces $p_{xz}(z)$ as a function of z calculated from three different block averages for polymer brushes at equilibrium and under shear ($\dot{\gamma}_a = 0.0001$ in reduced units)