Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronical Supporting Information for: Interaction strength between proteins and polyelectrolyte brushes: A small angle X-ray scattering study

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I. 2-DIMENSIONAL REPRESENTATION OF ALL INVESTIGATED SAMPLES BY SAXS

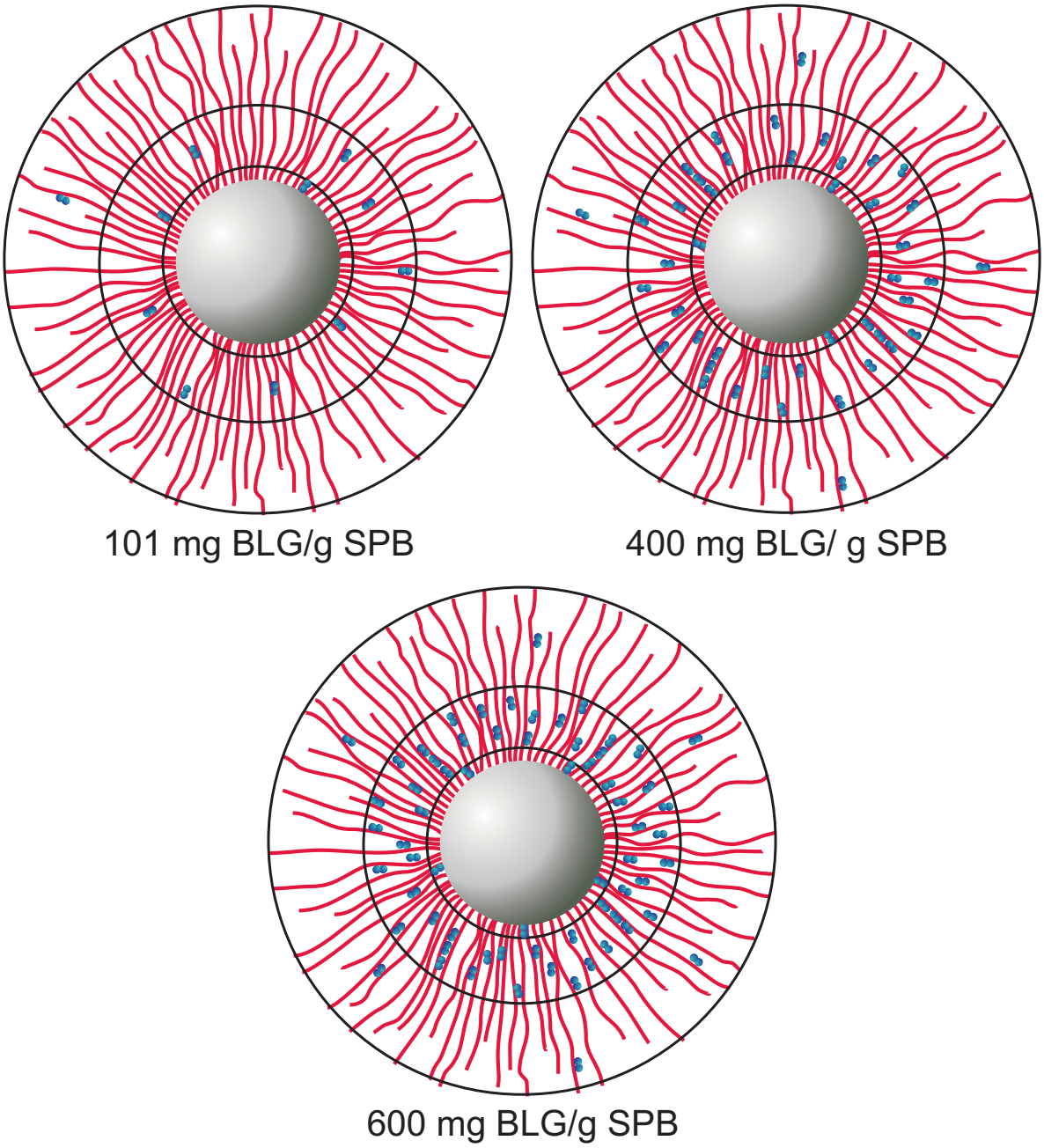

FIG. 1: 2-dimensional representation of the amount and distribution of BLG inside the brush layer derived from Fig. 2(a) of the publication from 101 to 600 mg BLG/g SPB. The protein molecules which are adsorbed in the outer part of the brush layer can be released by extensive ultrafiltration. The black lines represent the region of high and low protein adsorption.

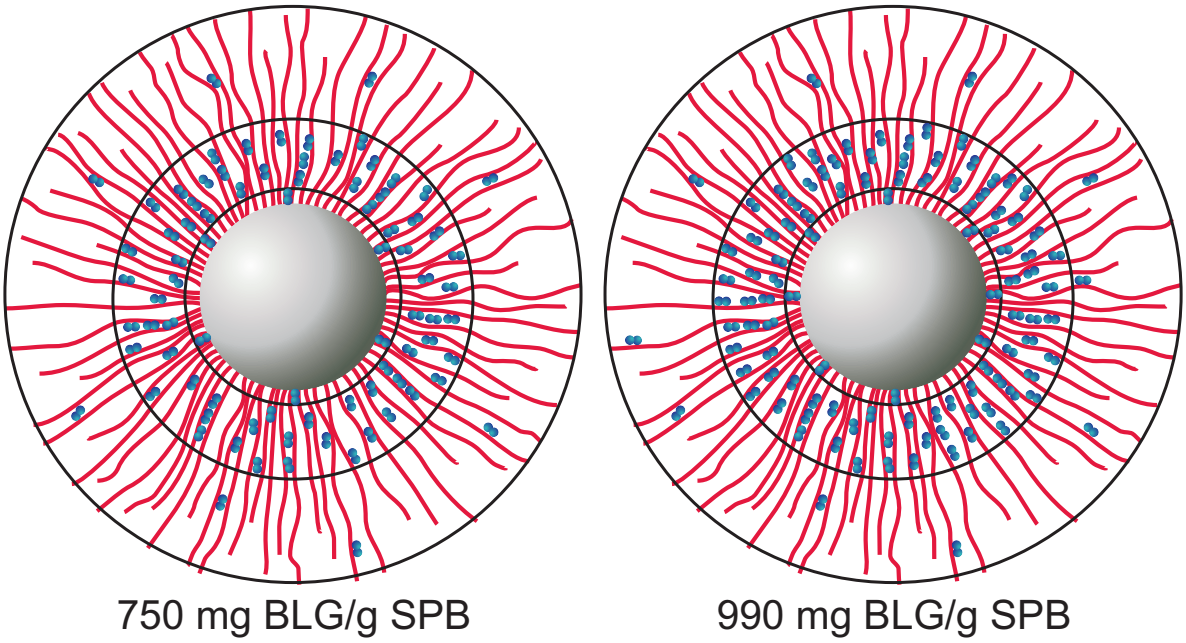

FIG. 2: 2-dimensional representation of the amount and distribution of BLG inside the brush layer derived from Fig. 2(a) of the publication from 750 and 990 mg BLG/g SPB. The protein molecules which are adsorbed in the outer part of the brush layer can be released by extensive ultrafiltration. The black lines represent the region of high and low protein adsorption.

II. TRANSFORMATION OF ITC DATA TO AN ADSORPTION ISOTHERM

The transformation of the isothermal titration calorimetry data (ITC) data to an adsorption isotherm starts from the considerations given in the paper. The ITC data were fitted by the software ORIGIN (Microcal, Northhampton, MA). The two sets of independent binding sites (TSIS) model is assumed. Each set of these binding sites has its own characteristic binding constant (K_{A1}, K_{A2}), molar heat of binding (ΔH_1, ΔH_2) and number of sites (N_1, N_2).[1] It is assumed that each binding site is independent from the other. Therefore, each type of site has its own fractional saturation (Θ_1, Θ_2). Thus, it is possible to define the binding constants for the two binding sites[1]

$$K_{A1} = \frac{\Theta_1}{(1-\Theta_1)\,[BLG]} \qquad K_{A2} = \frac{\Theta_2}{(1-\Theta_2)\,[BLG]} \tag{S 1}$$

where $[BLG]$ is the concentration of the unbound protein. The definition of the total concentration of β -lactoglobulin $[BLG]_t$ is given by[1]

$$[BLG]_t = [BLG] + [brush]_t \left(N_1\Theta_1 + N_2\Theta_2\right) \tag{S 2}$$

where $[brush]_t$ is the total brush concentration. Solving Eq. (S1) for Θ_1 respectively Θ_2 and substituting into Eq. (S2) gives

$$[BLG]_t = [BLG] + \frac{N_1 [brush]_t [BLG] K_{A1}}{1 + [BLG] K_{A1}} + \frac{N_2 [brush]_t [BLG] K_{A2}}{1 + [BLG] K_{A2}} \tag{S 3}$$

Solving of Eq. (S3) for $[BLG]$ leads to a cubic equation of the form[1]

$$\begin{aligned} 0 =& [BLG]^3 + k[BLG]^2 + l[BLG] + m \\ k =& \frac{1}{K_{A1}} + \frac{1}{K_{A2}} + (N_1 + N_2)[brush]_t - [BLG]_t \\ l =& \left(\frac{N_1}{K_{A2}} + \frac{N_2}{K_{A1}}\right)[brush]_t - \\ & \left(\frac{1}{K_{A1}} + \frac{1}{K_{A2}}\right)[BLG]_t + \frac{1}{K_{A1}K_{A2}} \\ m =& -\frac{[BLG]_t}{K_{A1}K_{A2}} \end{aligned} \tag{S 4}$$

The cubic equation can be solved in closed form if the parameters K_{A1}, K_{A2}, N_1 and N_2 are known. Therefore, the concentration of unbound protein can be calculated and the adsorption isotherm can be obtained.

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[1] L.-N. Lin, A. B. Manson, R. C. Woodworth and J. F. Brandts, *Biochemistry*, 1991, **30**, 11660.