

## Home assignments

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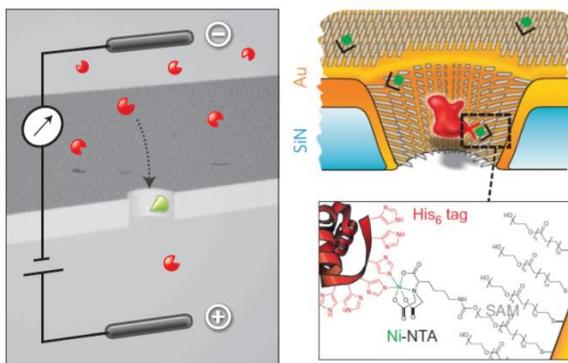
Virus capsids are shells of self-assembled proteins. Assume capsids that are approximately spherical with radius 30 nm are adsorbing irreversibly to a large planar surface from a large stagnant liquid. Each capsid consists of 120 proteins with molecular weight 40 kg/mol. The concentration of capsids is 10 µg/mL. How long time does it take to fill up the surface so that no more binding occurs?

Hint: When spheres bind to a surface in a random manner, the maximum areal coverage is 54.7%.

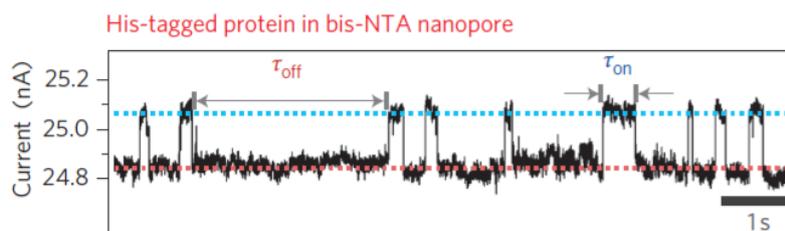
Assume water at room temperature. Get diffusion constant from Einstein-Stokes:  $D = k_B T / [6\pi\eta R] = 7.3 \times 10^{-12} \text{ m}^2/\text{s}$ . Each capsid has a weight of 4800 kg/mol, so the molar concentration is  $C_0 = 2.1 \times 10^{-6} \text{ mol/m}^3$ . The cross-section area of the virus is  $\pi R^2$  and 0.547 divided by this number is equal to  $\Gamma$  when the surface is filled (also divide with Avogadro's number), which gives  $\Gamma = 3.2 \times 10^{-10} \text{ mol/m}^2$ . Now use Ilkovic to solve for the time  $t = [\Gamma / [2C_0]]^2 \times \pi / D = 42 \text{ min}$ .

2

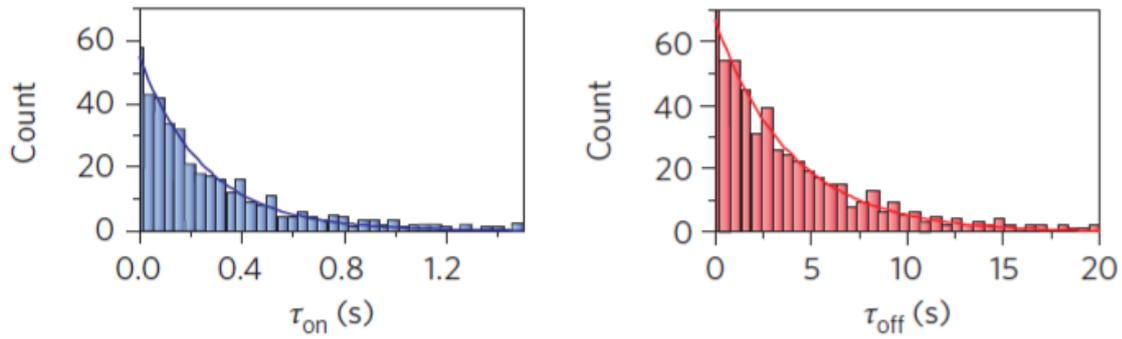
By measuring the ion current through single nanopores it is possible to make an extremely small sensor. When receptors are immobilized inside the pore it is possible that only a single receptor contributes to the sensor response:



Reversible binding and dissociation events can then be monitored and the sensor has two states. The following is an example of what the data can look like:



The events can be summarized in histograms. The following data is for 800 nM protein concentration in solution:



Estimate the dissociation constant of the interaction! (Figures from Wei et al. *Nature Nanotechnology* 2012, 7 (4), 257-263.)

We need  $k_{\text{on}}$  and  $k_{\text{off}}$ . When a molecule is bound the distribution of times until dissociation should follow an exponential decay just like in an ensemble average measurement. The right curve has decreased by a factor  $1/e$  at  $\sim 4$  s and thus  $k_{\text{off}} = 1/4 \text{ s}^{-1}$ . For the association the principle is the same, i.e. exponential decay of probability distribution for time until the event occurs, but we need to include the concentration. The curve has decreased by a factor  $1/e$  at  $\sim 0.3$  s and thus  $k_{\text{on}} = 1/[0.3 \times 800 \times 10^{-9}] \approx 4.16 \times 10^6 \text{ s}^{-1} \text{ M}^{-1}$ . This gives  $K_D = k_{\text{off}}/k_{\text{on}} = 60 \text{ nM}$ .