Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2017

Supporting Information

Geometrical parameters of the hyperboloid

The one-sheet hyperboloid is a quadric with equation 4 in the main text and reported here for sake of completeness.

$$\left(\frac{x'}{a}\right)^2 + \left(\frac{y'}{b}\right)^2 = 1 + \left(\frac{z'}{c}\right)^2 \quad (S1)$$

The central section of the hyperboloid, i.e. $z' = 0$ in Eq. S1, defines the ellipse with equation

$$\left(\frac{x'}{a}\right)^2 + \left(\frac{y'}{b}\right)^2 = 1 \qquad (S2)$$

with a and b the length of the ellipse semi-axes along the x' and y' axes, respectively. Note that the hyperboloid axes are in general not coincident with the GROMACS Cartesian reference system (x,y,z), i.e. all hyperboloid geometrical parameters are expressed in the internal reference frame of the hyperboloid x', y', and z'.

The sections sliced by the $x' = 0$ and $y' = 0$ planes are the hyperbolas:

$$\left(\frac{y'}{b}\right)^2 - \left(\frac{z'}{c}\right)^2 = 1 \qquad (S3)$$

$$\left(\frac{x'}{a}\right)^2 - \left(\frac{z'}{c}\right)^2 = 1 \qquad (S4)$$

respectively. Planes with equation $z' = k$ intercept the hyperboloid, producing the ellipse

$$\left(\frac{x'}{a}\right)^2 + \left(\frac{y'}{b}\right)^2 = 1 + \left(\frac{k}{c}\right)^2 \qquad (S5)$$

with semi-axes lengths

$$a' = \frac{a}{c}\sqrt{c^2 + k^2} \qquad (S6)$$

$$b' = \frac{b}{c}\sqrt{c^2 + k^2} \qquad (S7)$$

respectively. We can now define the three-dimensional pore surface as a one-sheet hyperboloid: I) a and b can be evaluated by the numerical characterization of the central ellipse given in Eq. S2; II) c can be evaluated with the same procedure, by taking into account two k values in Eq. S5 suitable for identifying the hyperboloid (electropore) lower and upper ellipses, and then extracting c via Eqs. S6 and S7.

In the main text we identified the proper values for the k parameters, and hence the length of the pore along its axis, by considering the probability distributions of nitrogen atoms on the lipid head groups along the z-axis of the Cartesian reference frame.

The electropore terminations (ends) have been chosen by taking into account $k = +1$ and $k = -1$, i.e. symmetrically placed with respect to the center of the nitrogen atoms probability distribution.

From the time-series of the semi-axes associated to the central ellipse (see Figure S1, panel B) and lower and upper ellipses (see Figure S1, panel C and D) we can evaluate the mean values for a, a', b, b'

to be used in eqs. S5, S6 and S7 to evaluate the c parameter and, eventually, the complete analytical form of the one-sheet hyperboloid.

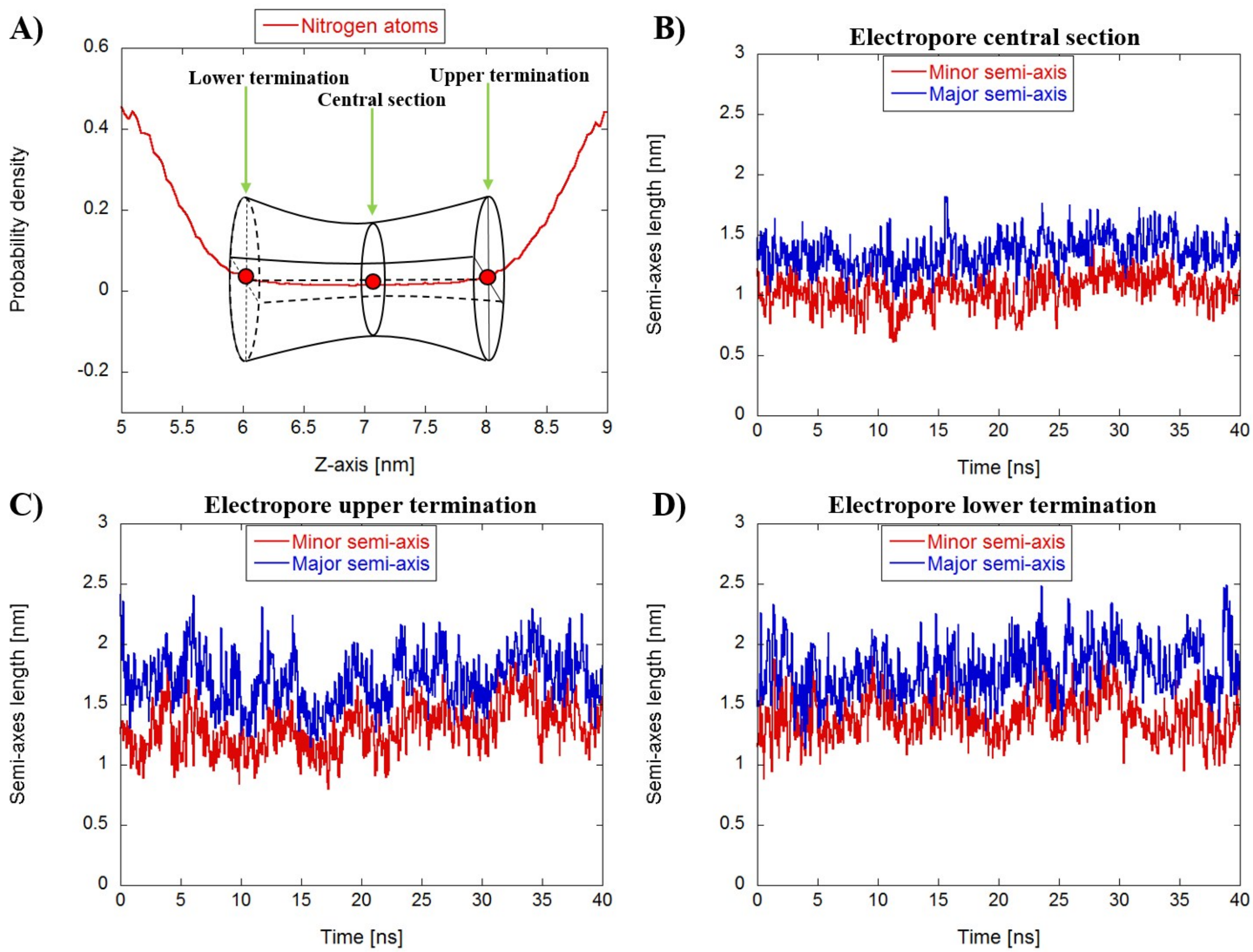

Figure S1. Panel A shows the probability distribution of the nitrogen atoms. The two Gaussian-like peaks (centered in 5 and 9 nm along the z-axis) correspond to the two interface regions of the bilayer. The non-zero nitrogen density, in the interval between 6 nm and 8 nm, comes from the head groups forming the pore wall. The electropore terminations (ends) can be properly chosen by taking into account z' values inside the inner region. Here about 5% of the distribution peaks for both ends of the pore were used. Panels C, D and E show the stability over time of the lengths of the minor and major axes of the three ellipses defining the pore

Table S1 shows the axes lengths for the central section of the pore, the upper and lower electropore terminations, respectively, together with their standard errors (evaluated by using 5 different portions of the total trajectory). It is apparent from the table that the measures of the upper and lower ellipses are essentially the same (within the standard error), hence the application of eq. S6 or S7 gives an unambiguous result for the c parameter, precisely $c = 1.22$ nm.

Table S1

Elliptic section	Central section	Upper termination	Lower termination
Major axis [nm]	1.35 ±0.02	1.74±0.04	1.79±0.03
Minor axis [nm]	1.03±0.03	1.33 ±0.05	1.39 ±0.03

The knowledge of all the parameters needed in eq. 1 allows the explicit surface representation of the hyperboloid, shown in Figure S2, obtained via Mathematica software (v8.0)

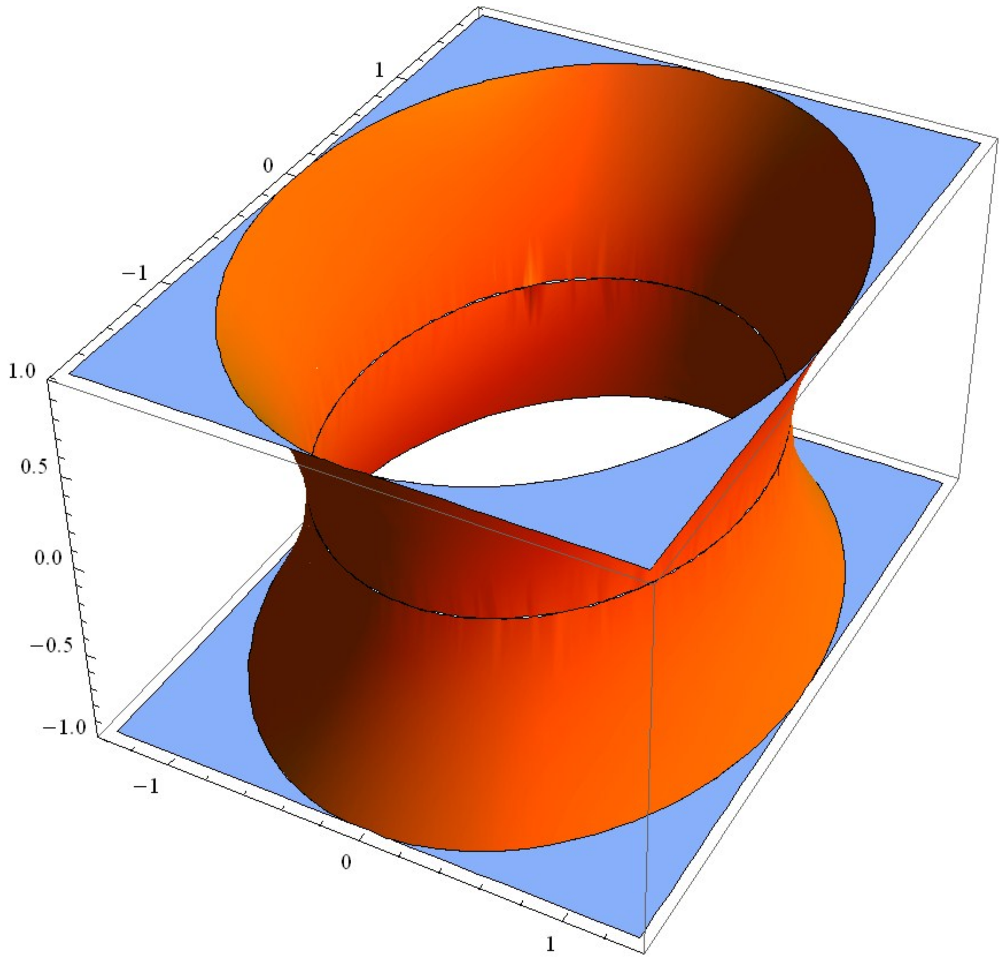

Figure S2 The one-sheet hyperboloid as obtained with the following parameters [$a = 1.03$ *nm;* $b = 1.35$ *nm;* $c = 1.22$ *nm;* $a' = 1.33$ *nm;* $b' = 1.74$ *nm].*