Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Tunning the Transdermal Transport by External Continuous Electric Field Application: A Molecular Dynamics Coarse-Grained Mechanism for Iontophoresis

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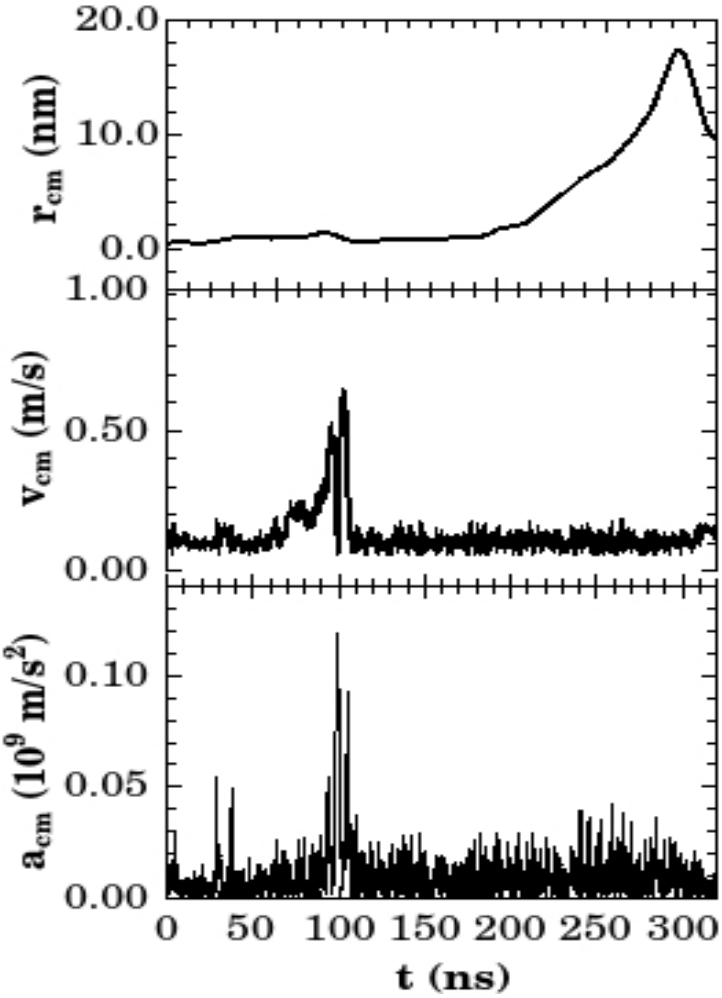

Figure S1: Center of mass position (a), velocity (b) and aceleration (c) for vesicle formation under 22.8 mV/nm electric field.

Contributions of electrostatic images

We estimate the contribution due to the electrostatic images from the central super-cell using the results of ref. RS1 . The effective field E_z^{eff} experienced by the vesicle in the interface will be

$$E_z^{eff} = E_z^0 + E_0^{ind}$$

where E_z^0 and E_0^{ind} are the applied and induced electric fields, respectively. The induced electric field is given by $E_0^{ind} = \frac{k_e \langle M_z \rangle}{4\pi V}$, where k_e is the Coulomb constant, V the volume, and h $\langle M_z \rangle$ i the average electric dipole along z-axis of the box. By including a finite layer of vacuum in the top and bottom sides of simulating box (see inset of Fig.S2) it is possible to smear out the long range electrostatic interactions. The relative relevance of the electrostatic images would be estimated by computing the induced to applied electric field ratio E_0^{ind}/E_z^0 as function of the increasing vacuum layer thickness of the simulation box (h). Were simulated 23 boxes with $0 \leq h \leq 60$ nm using the start coordinates for the calculation of $\langle M_z \rangle$. For these simulations, the comprehensibility along the z-axis direction was set to zero. The other parameters remained the same.

Figure S2 presents E_0^{ind}/E_z^0 as function of the vacuum layer thickness for E_z^0 = 7 mV/nm. The strongest dependency appeared for vacuum layer < 20 nm. Typically $E_0^{nnd} \sim -10^{-3} E_z^0$. In fact, it was reported that some degree of water viscosity anisotropy induced due to electric field occurs for $E_z^0 \sim 0.2$ V/nm. [RS2] This field is 5 orders of magnitude greater than our E_z^0 applied value. Thus it is possible to state that in our case the effective field experienced by the system, water in particular, will not be able to induce appreciable changes in the water content properties.

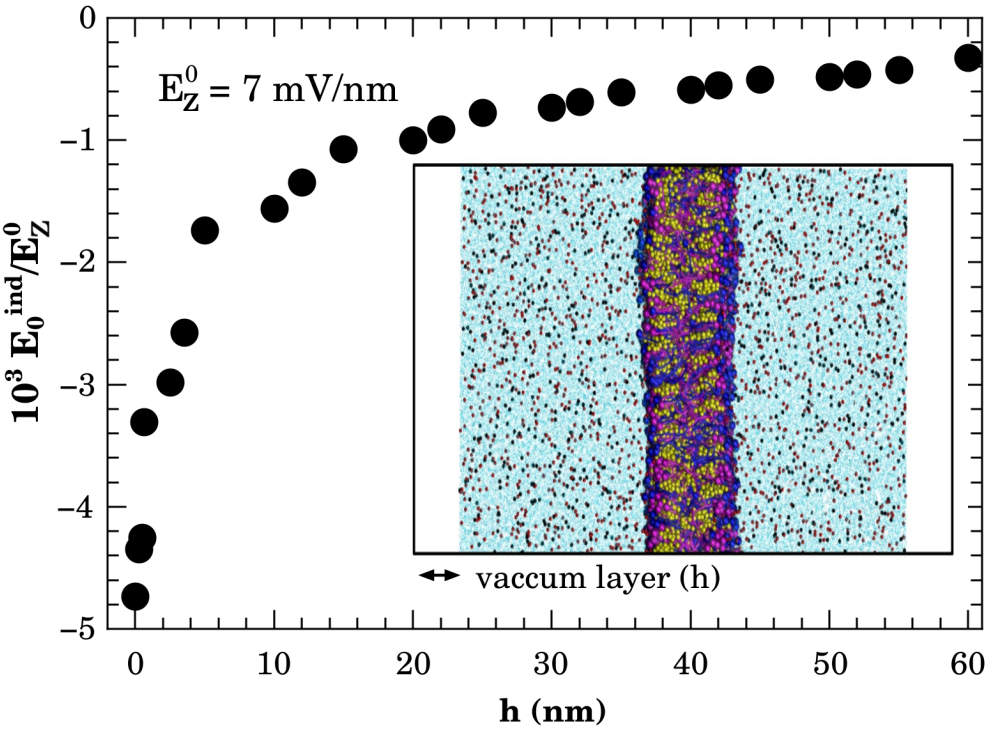

Figure S2. Induced to applied electric field ratio (E_0^{ind}/E_z^0) as function of the vacuum layer thickness of the simulation box (see inset) for E_z^0=7 mV/nm.

Radius of gyration

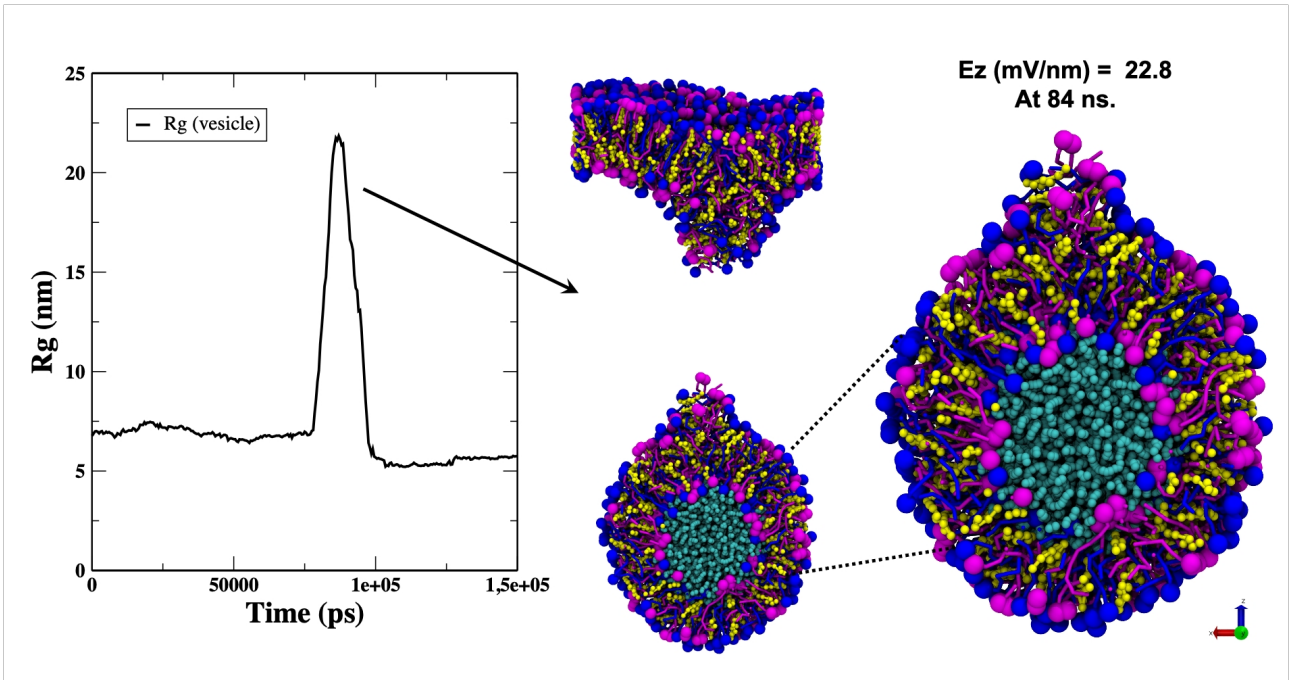

Figure S3. Time dependency (left) of radius of gyration (Rg) showing the instant of vesicle detachment from membrane. The secion view (right) shows details of internal vesicle composition and structure.

References

[RS1] I.-C. Yeh and M. L. Berkowitz, J. Chem. Phys., 1999, 111, 3155–3162.

[RS2] D. Zong, H. Hu, Y. Duan and Y. Sun, J. Phys. Chem. B, 2016, 120, 4818–4827.