# Electronic Supplementary Information: Electrostatic interaction between SARS-CoV-2 virus and charged electret fibre

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## I. CHARGE REGULATION PARAMETERS

To determine the charge on the S proteins, we first extract solvent-accessible ionizable amino acids (AA) from the structural data in PDB:6VXX [1]. We consider deprotonated (ASP, GLU, TYR, and CYS) and protonated (ARG, LYS, and HIS) AAs, whose solvent accessibility is determined using propKa 3.1 [2]. Only those AA residues that are buried less than 80% are kept and considered to carry any charge [3]. This retains 504 out of 702 ionizable AA residues, and the detailed composition by residue type is given in Table SI. Given the general coarse-grained nature of our model, we attribute to each AA functional group its $\mathrm{pK_a}$ value in bulk dilute aqueous solution. The values in Table SI are then used in Eq. (2) in the main text together with any local electrostatic potential to obtain the charge-regulated surface charge distribution on the model S proteins.

Table SI. Charge regulation parameters for the surface of S proteins. For each deprotonated ($q_\pm = -1\ e$) and protonated ($q_\pm = +1\ e$) AA functional group we use their $\mathrm{pK_a}$ value in bulk dilute aqueous solution, taken from Ref. [4]. The number of ionizable, solvent-accessible amino acid residues $N_S$ on the S protein is obtained from structural data PDB:6VXX.

| AA | $q_\pm$ [$e$] | $\mathrm{pK_a}$ | $N_S$ |
|---|---|---|---|
| ASP | $-1$ | 3.71 | 123 |
| GLU | $-1$ | 4.15 | 84 |
| TYR | $-1$ | 10.10 | 84 |
| CYS | $-1$ | 8.14 | 3 |
| ARG | $+1$ | 12.10 | 63 |
| LYS | $+1$ | 10.67 | 120 |
| HIS | $+1$ | 6.04 | 27 |

## II. ELECTROSTATIC POTENTIAL

The local electrostatic potential is obtained as a solution of the PB equation [Eq. (3) in the main text] in the regions accessible to the bathing solution (external solution accommodating the virus as well as the virus interior) and the Poisson equation in the inaccessible regions (membrane envelope, S protein cores, and the electret substrate), with boundary conditions given by Eq. (4) in the main text. Since the surface charge density on the S proteins is obtained from the charge regulation model, it varies spatially along the surface; on the other hand, the surface charge density on the electret is assumed to be fixed. Example in Fig. S1 shows a two-dimensional cross-section of the local electrostatic potential around the virus in the absence of the electret substrate, i.e., for an isolated virus.

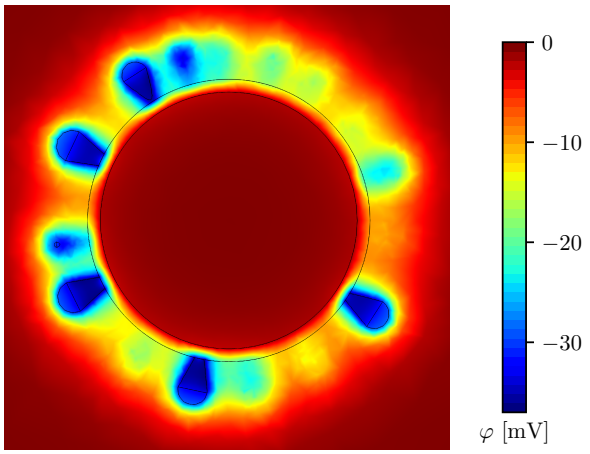


Figure S1. Two-dimensional cross-section of the model, showing the local electrostatic potential $\varphi$ of a virus with $N = 80$ S proteins in the absence of the electret surface, with $n_0 = 2$ mM and pH = 7. Black circles show the inner and outer surface cross-sections of the lipid membrane, which carry no charge.

## III. MAXWELL AND OSMOTIC COMPONENTS OF THE TOTAL ELECTROSTATIC FORCE

Based on the standard PB theory [5], the stress tensor anywhere within the bathing ion solution can be decomposed into Maxwell and van't Hoff components, corresponding to the field stresses and the salt ion osmotic pressure, respectively [Eq. (5) in the main text]. The total force on a body within the bathing solution is then obtained by integrating the stress tensor over any closed surface containing the body. Numerically, it is best to choose an integration surface that is finely meshed to ensure a high numerical accuracy of the result, and to obtain our results, we have consistently chosen the surface next to the epitope of the virus.

The relative contributions of Maxwell and van't Hoff components to the total stress tensor—and consequently to the total interaction force—vary with the external parameters. Figure S2 shows the total electrostatic force on the virus as a function of its distance from the electret surface together with its decomposition into the electrostatic component from the Maxwell stress tensor and the osmotic component. When the net force is attractive, the Maxwell component clearly dominates, whereas when the net force is repulsive, the contributions of the Maxwell and van't Hoff terms are comparable, regardless of the sign of the surface charge density on the electret fibre.

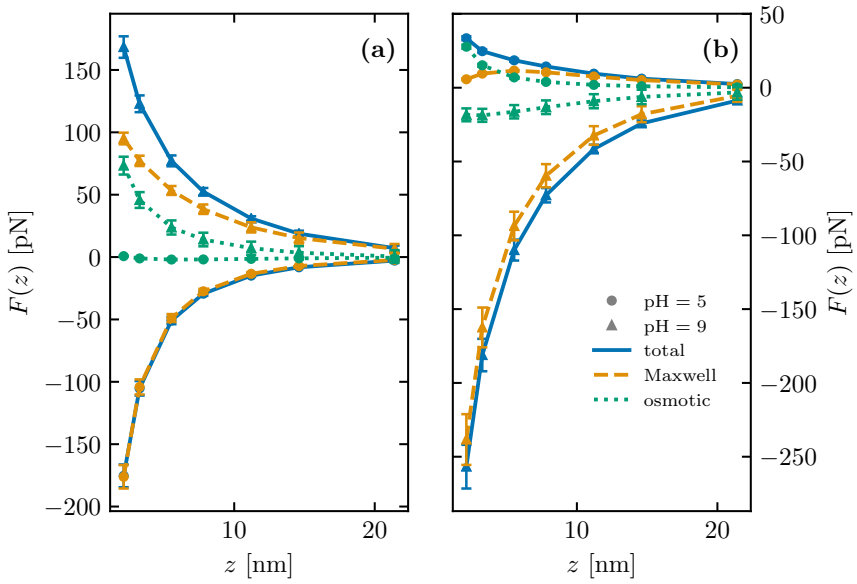


Figure S2. Total electrostatic force on the virus and its Maxwell (electrostatic) and osmotic components as a function of distance from the electret surface, for a system with $N = 80$, $n_0 = 2$ mM, and **(a)** $\sigma_S = -1\ e/\text{nm}^2$ and **(b)** $\sigma_S = +1\ e/\text{nm}^2$. The legend is the same for both panels. Shown are also the errorbars, obtained by averaging over approximately 20 different Mitchell configurations of S proteins on the surface of the lipid membrane for each data point.


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