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

Supporting Information: Electromechanics of the liquid water vapour interface

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The choice of the dividing surface between interface and bulk regions

In the Main Text, the dividing surface is chosen as 0.9 nm from the onset of $\gamma_T(z)$ profile which includes the topmost three layers of water molecules at the water vapour interface.

Here, we show how the choice of the dividing surface affects the outcome of the response of γ_T with respect to the D field.

In Fig. S1, the dividing surface is chosen as 0.6 nm instead. The main feature as shown in Fig. 3 in the Main Text, a concave and asymmetric parabola, remains. However, one needs to notice that the γ_T at $D = 0$ is far below the macroscopic surface tension which is 610 bar*nm. This means the choice of the dividing surface as 0.6 nm falls short of including all interfacial contributions.

In Fig. S2, the dividing surface is chosen as 1.2 nm. The shape of a concave and asymmetric parabola starts to deteriorate which indicates the mixing of interfacial and bulk regions. In constrast to that in the interfacial region, the bulk response is a convex and symmetric parabola, as shown in Fig. 4 in the Main Text.

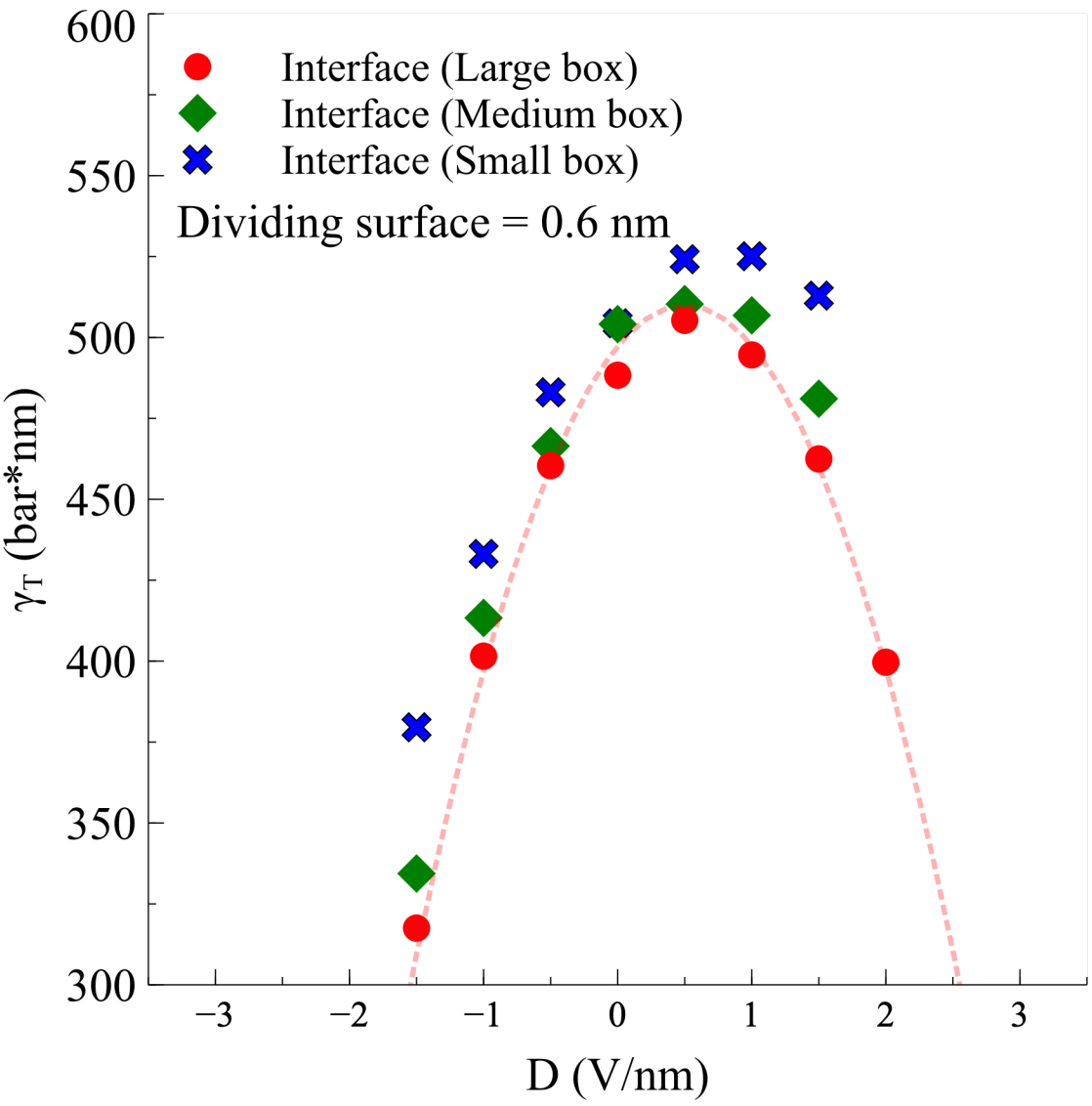

Figure S1: Field-dependent tangential component γ_T of the surface tension of the liquid water vapour interface. L_z=5.55 nm, 8.33 nm and 11.11 nm are the values for the length in the direction normal to the surface for a small, medium and large MD box respectively. A dividing surface is chosen as 0.6 nm.

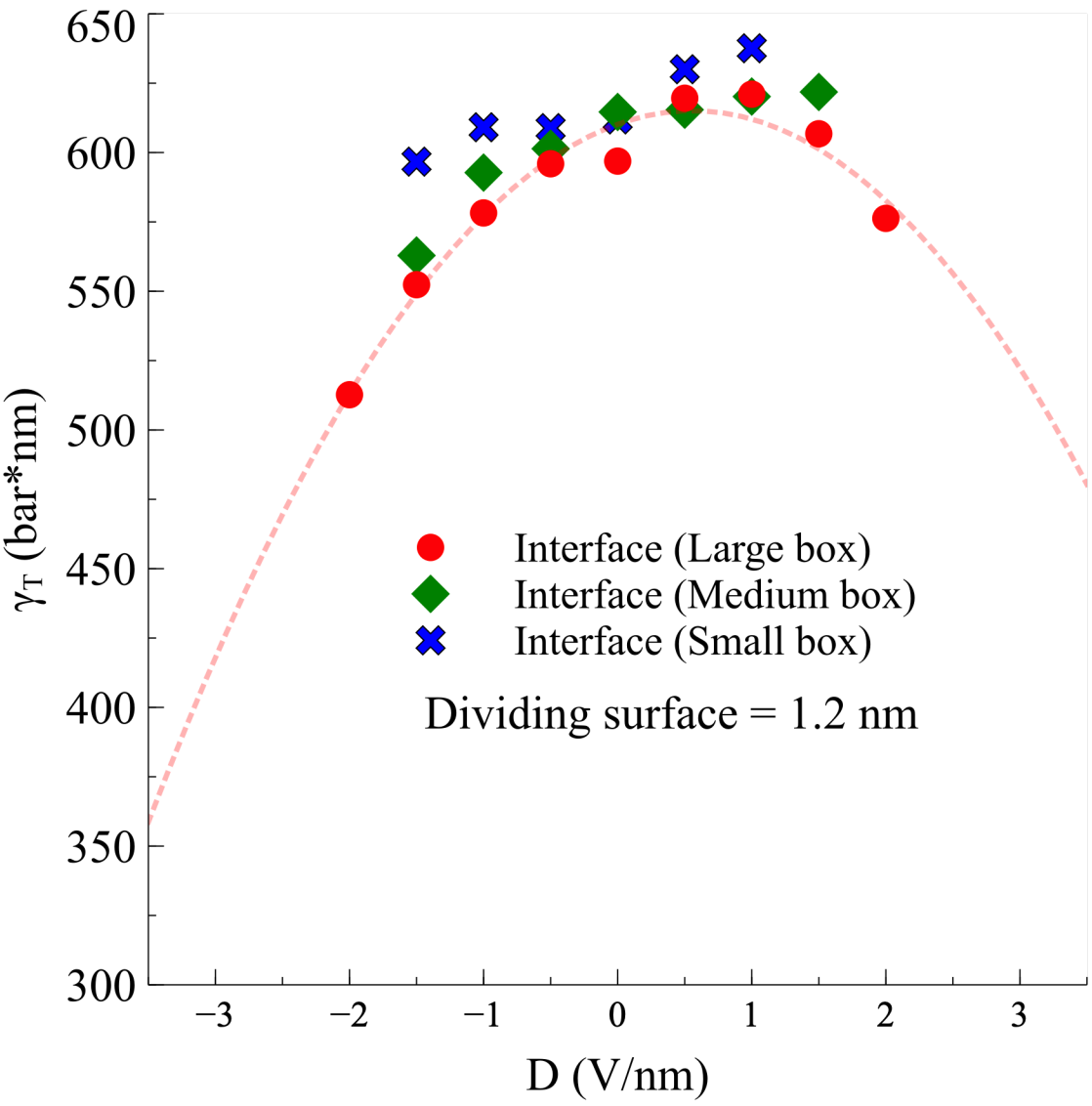

Figure S2: Field-dependent tangential component γ_T of the surface tension of the liquid water vapour interface. L_z=5.55 nm, 8.33 nm and 11.11 nm are the values for the length in the direction normal to the surface for a small, medium and large MD box respectively. A dividing surface is chosen as 1.2 nm.