<u>Supporting Information</u>

Electric charge induced active control of nucleate and rapid film boiling at nanoscale: a molecular perspective

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Supplementary information for electric charge assisted explosive boiling on surface A.

For the results shown in Fig. 2(a), the representative snapshots of simulation are presented in Figure S1 with electric charge intensities of 0.006e and 0.012e.

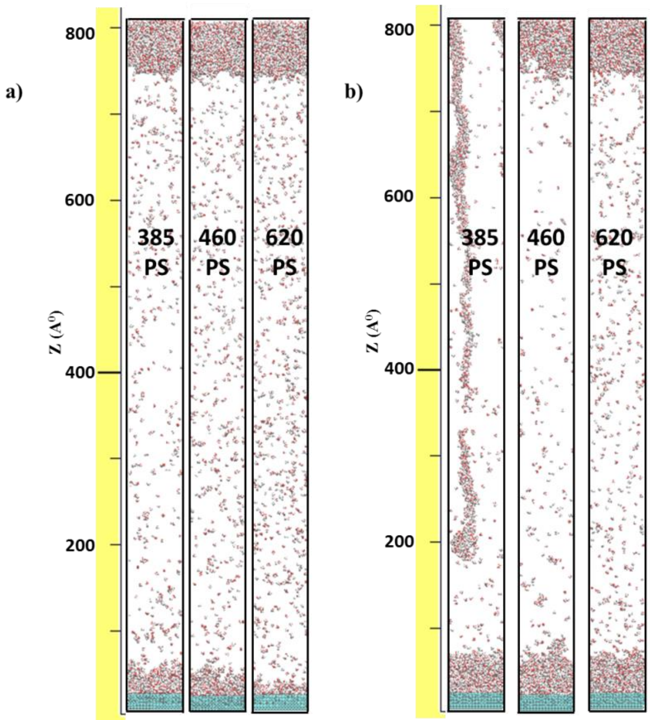

Figure S1. Snapshot of simulation of rapid boiling when surface is maintained at temperature of 700 K with electric charge intensity (a) 0.006e (b) 0.012e

Supplementary information on electric charge assisted explosive boiling on Surface B

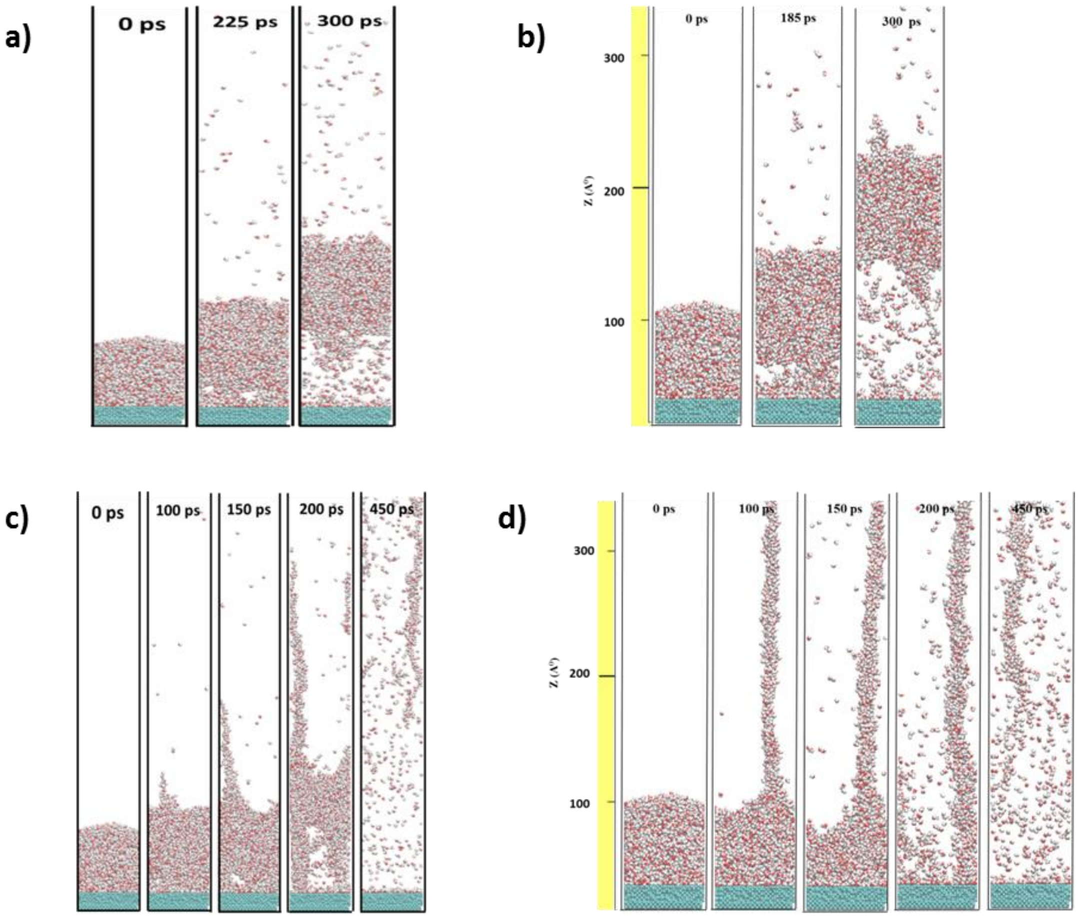

Figure S2. Snapshots of simulation on surface B with surface temp 700 K and electric charge intensity (a) E = 0 (b) E = 0.017e (c) E = 0.02e (d) E=0.025e

The snapshots of the simulation on surface B have been shown in Fig. S2. In this case, the phenomenon of rapid boiling with only heat appears to be the same as seen before (Fig. S2(a)) with associated volume expansion, nucleation formation (at 225 ps), and vapour film formation near the surface leading to complete detachment of liquid film (300 ps). The only difference is that the rapid boiling happens much faster in the case of hydrophilic surfaces than the non-wetting surface, where we have observed liquid film detachment much later (at about 585 ps, Fig. (1b)). This is because; on hydrophilic surface, solid-liquid interaction will be higher (because of increased wettability) due to which there will be increased heat transfer rate between surface and water film resulting in faster explosive boiling. This observation is consistent with other molecular simulations available in literature.[1,2] In the case of electric field-induced rapid boiling on the hydrophilic surface (Surface B), a distinct phenomenon has been observed as compared to the non-wetting surface (Surface A). On surface B, for electric charge intensities lesser than 0.02e, no water column formation was seen. The water film was observed to completely detach from the surface, similar to rapid boiling with only heat (Fig S1(b)). Figure S1(c) shows the snapshots of simulation when surface B is charged with an electric charge of 0.02e. In this case, the water column formation has been observed to happen along with volume expansion as opposed to water film thinning down as observed in the case of non-wetting surface (Fig. S1(a)). The nucleation is observed to start at about 150 ps, and even as the bubble grows (200 ps) and breaks through, the water film is not observed to detach from the surface. At 450 ps, complete boiling of the liquid film can be seen in Fig. S1(b). Simulations have also been done with higher electric charge intensity of 0.025e (Fig. S1(c)), and a similar phenomenon as seen in Fig. S1(b) has been observed but with faster water column growth, nucleation, and complete boiling process.

Figure S3 shows the probability distribution curve of the angle of water molecules at 150 ps for different electric charges. It can be observed from the figure that there exists not much change in the distribution curves at E= 0 and E =0.017e, which supports that not much change in orientation of water dipole takes place at the lesser electric field, and hence no water column formation has been observed at lower electric charges. As the intensity is increased, a shift in the peak of the curve to smaller angles can be seen, which is due to the change in orientation of water molecules in the direction of the applied field resulting in water column formation. In the case of a hydrophilic surface, the water column growth rate has been observed to increase as the charge intensities are increased. This can also be confirmed by comparing the snapshots of simulation at 150 ps for different electric charges provided in the inset of Figure S3.

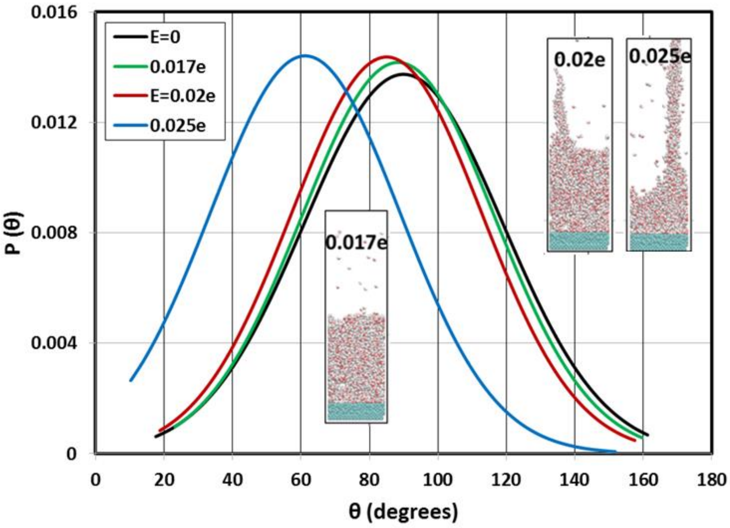

Figure S3. The probability distribution of angle of water molecules under different charge on surface B

Energy density calculation

Energy density for rapid boiling is calculated as total energy per unit volume added to the liquid film till a vapour layer is formed near the surface and a complete detachment of water film takes place. The same during explosive boiling at different surface temperatures is shown in Table A1. One can note that the calculated energy density needed for explosive boiling is of a similar order as compared to the experimental observations in the literature (8.46×10^8 J/m^3; Elias and Chambre,[32] and $8.5 \times 10^8 - 10.2 \times 10^8$ J/m^3; Hassan et al.[33]).

Table A1 Energy density needed for explosive boiling at different surface temperatures

Surface temperature (K)	Energy Density (J/m^3)
700	8.802×10^8
800	9.298×10^8
900	9.44×10^8
1000	9.56×10^8

References for supporting information

(1) Wang, B.-B.; Wang, X.-D.; Wang, T.-H.; Lu, G.; Yan, W.-M. Enhancement of Boiling Heat Transfer of Thin Water Film on an Electrified Solid Surface. *Int. J. Heat Mass Transf.* **2017**, *109*, 410–416. https://doi.org/10.1016/j.ijheatmasstransfer.2017.02.029.

(2) Bai, P.; Zhou, L.; Du, X. Effects of Surface Temperature and Wettability on Explosive Boiling of Nanoscale Water Film over Copper Plate. *Int. J. Heat Mass Transf.* **2020**, *162*, 120375. https://doi.org/10.1016/j.ijheatmasstransfer.2020.120375.